

Numerical methods for the fractional Laplacian and related nonlocal PDEs



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To my family.

The beauty of it smote his heart, as he looked up out of the forsaken land, and hope returned to him. For like a shaft, clear and cold, the thought pierced him that in the end the Shadow was only a small and passing thing: there was light and high beauty for ever beyond its reach.

J.R.R. Tolkien (1892–1973), “The Lord of the Rings”

Tomorrow will be the 22nd century.

Nina Simone (1933–2003), “22nd Century”

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Abstract

The thesis develops and analyses finite element methods for the fractional Laplacian and related partial differential equations. Our work spans rigorous numerical analysis and scientific computing, addressing evolutionary diffusion problems and elliptic boundary value problems, studying numerical methods for the fractional Laplacian on bounded domains in both its spectral and integral definition.

A central contribution of the initial part of the thesis is the construction of the first provably convergent finite element scheme on a bounded domain for a parabolic regularisation of the porous medium equation with a fractional pressure. The model consists of a nonlinear diffusion equation in which the pressure is determined through the spectral fractional Laplacian with a Neumann boundary condition. The convergence proof also constitutes a constructive existence argument for weak solutions, while the scheme preserves mass conservation, nonnegativity of the density, and the free energy dissipation structure of the continuous problem. The analysis is then extended to a broader class of porous medium equations involving spectral fractional powers of second order elliptic operators, incorporating anisotropy and confinement. On the computational side, the thesis develops an efficient algorithm for the spectral fractional Laplacian based on rational approximation theory, circumventing the high computational cost of full spectral decompositions. This is used to perform the first study of the fractional Keller–Segel equation on bounded domains from a computing perspective, exploring blow-up phenomena and their dependence on mass and concentration of the initial datum.

We then study the integral fractional Laplacian on a bounded domain and a classical elliptic problem associated with it. In this context, the thesis proposes a finite element method with a weighted basis that exploits the known low regularity of solutions near the boundary, by incorporating this directly into the scheme, through a finite element basis having the same (low) regularity. Under natural regularity assumptions on the domain, the method is shown to improve all previously known error estimates in the fractional Sobolev norm. A companion quadrature rule for the resulting nonlocal bilinear form is also developed. The quadrature, efficiently computable through the use of the Riemann and Epstein zeta functions, enables a systematic study of the interplay between finite element discretization and bilinear form approximation for the finite element method with a weighted basis and comparison with the standard piecewise linear basis.

Taken together, the thesis makes original contributions to the rigorous numerical analysis of nonlocal PDEs, to the design of practically implementable algorithms, and to the mathematical understanding of fractional nonlocal diffusive processes on bounded domains.

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List of Symbols

$\delta_{i,j}$	Kronecker delta of indices i and j
$\text{span}\{v_1, \dots, v_n\}$	linear span of vectors $v_1, \dots, v_n$
$B_r(x)$	ball of radius r centred at x
B_r	ball of radius r centred at zero
$\overline{\Omega}$	closure of a set Ω
Ω°	interior of a set Ω
$\partial/\partial x_i$	(weak) derivative in the i -th variable
$(\partial/\partial x)^\alpha$	(weak) derivative of multi-index $\alpha = (\alpha_1, \dots, \alpha_d)$
$C_0^\infty(\mathbb{R}^d)$	space of smooth functions in $\mathbb{R}^d$ with compact support
$C_b(\mathbb{R}^d)$	space of bounded continuous functions in $\mathbb{R}^d$
$L^p(\Omega)$	Lebesgue space of summability p in a domain Ω
$W^{k,p}(\Omega)$	Sobolev space of order k and summability p
$H^k(\Omega)$	Sobolev space of order k and summability 2
$H_0^1(\Omega)$	Sobolev space of functions in $H^1(\Omega)$ with zero trace on $\partial\Omega$
$H_*^1(\Omega)$	Sobolev space of functions in $H^1(\Omega)$ with zero average on Ω
$\mathcal{F}$	Fourier transform
$(-\Delta)^s$	fractional Laplacian of order s
$(-\Delta_{\mathcal{B}})^s$	spectral fractional Laplacian of order s , boundary condition $\mathcal{B}(\cdot)$
$(-\Delta_{\text{D}})^s$	spectral fractional Dirichlet Laplacian of order s
$(-\Delta_{\text{N}})^s$	spectral fractional Neumann Laplacian of order s
$H^s(\mathbb{R}^d)$	fractional Sobolev-Slobodeckii spaces of order s
$a_s(\cdot, \cdot)$	bilinear form associated to the integral fractional Laplacian
$\mathbb{H}^s(\Omega)$	domain of the spectral fractional Laplacian on a domain Ω
$\mathcal{T}_h$	triangulation of a domain
$(-\Delta_h)^s$	finite dimensional spectral fractional Laplacian

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Introduction

“Ainsi il s’ensuit que $d^{\frac{1}{2}}x$ sera égal à $x\sqrt{dx} : x$. Il y a de l’apparence qu’on tirera un jour des conséquences bien utiles de ces paradoxes, car il n’y a guères de paradoxes sans utilité.” (“Thus it follows that $d^{\frac{1}{2}}x$ will be equal to $x\sqrt{dx} : x$. It appears that one day useful consequences will be drawn from these paradoxes, for there are hardly any paradoxes without utility.”)

This was the answer by G. W. Leibniz directed to G. A. l’Hôpital in what it is historically considered the first mention of fractional calculus in an epistolary exchange between the two of them [132, letter 30 September 1695]. Since then, knowledge of fractional calculus has advanced significantly and different contributions have brought to rich mathematical formulations, that still constitute a lively area of research from both a theoretical and applied point of view.

The area of research of the current doctoral thesis is the study, from a numerical analysis perspective, of Partial Differential Equations (PDEs) that involve fractional powers of elliptic operators, mainly the fractional Laplacian. More precisely, the focus of the work is the design of numerical schemes, based on Finite Elements (FE), for different types of PDEs and for approximation of the fractional operators that are involved. The study examines elliptic and parabolic problems with the aim of providing novel numerical methods in different contexts.

The main scientific contributions of the doctoral thesis are several. In the first place we study a class of evolutionary PDEs involving fractional operators and we propose a numerical scheme for them, with a rigorous proof of convergence for the resulting numerical approximations. These equations, that will be derived in the following chapter, have the form

$$\frac{\partial \rho}{\partial t} = \Delta \rho - \nabla \cdot (\rho \nabla c),$$

where the term c will depend on ρ through the use of fractional operators.

On the one hand, the novelty of this part of work lies in the finite element framework that allows the construction of reliable and mathematically justified numerical approximations. On the other hand, we explore computationally different configurations of these models for the first time, using state-of-the-art algorithms and solvers to produce simulations and validate properties of the numerical scheme. Hence, the numerical analysis for the evolutionary PDEs under consideration offers interesting mathematical techniques, advanced scientific computing for fractional operators, and valuable insights through accurate and rapid simulations.

In addition to these contributions, we also propose a novel finite element scheme for a classical elliptic problem involving a particularly challenging definition of the fractional Laplacian. We develop a theory for a tailored finite element basis and, with this new method, under some assumptions on regularity of data and domain, we theoretically prove improvements of previous error estimates available in the literature. Furthermore, we validate computationally the increase in the speed of convergence with a robust software.

We begin by motivating the use of fractional operators in PDEs and their capability in terms of applications. Some of the PDE models that we are going to analyse are diffusion models that describe the evolution in time of the spatial distribution of densities, generally representing particles (whether they are electric charges, biological cells, or fluid molecules) on a specific region of space. Classical mathematical models for diffusion processes are often based on the use of differential operators to describe the spreading of the particles of the system. By definition, using classical differential operators, these models assume that the density of particles that is being modelled involves only local interactions between the particles themselves. This assumption however need not always be valid. From biology to physics there are several examples of particles for which it is reasonable to assume a nonlocal interaction among them while they move in space: growth of bacteria [140, 10], movement of antibodies [121, 134], crystal dislocation [90], human travel [150], electromagnetic fluids [177] are all examples for which long range interactions could be a realistic feature to assume. Nonlocal interactions often lead to superdiffusive phenomena, or in other words long-range spreading. The quest for a mathematical framework able to model diffusion processes, while taking into account nonlocal interactions, has motivated a large part of recent research in analysis of nonlocal PDEs. Interestingly, fractional calculus constitutes an example of such a mathematical formulation capable of incorporating a type of nonlocality and providing a valuable path to answer some of these needs. The application of fractional calculus to PDEs is both rich from a mathematical point of view and versatile from an applied perspective. The literature on fractional models is large and we refer the reader to [127] for a recent general discussion on the topic, [128] for application in physics, biology and medicine and to [171] for a rigorous discussion of fractional diffusion models. As we said previously, the most famous and widely studied operator that we will consider for our study is the fractional Laplacian. The use of the fractional Laplacian in super-diffusive processes is discussed in a large body of literature and the reader may wish to refer to [9, 71, 99] for some examples of its application. We cite also [10, 135] as two explanatory examples in which super-diffusion given by the fractional Laplacian is detected respectively in real bacteria swarming and in the navigation of a photosensitive alga.

The aim of the introduction is to provide a brief summary of the mathematical background for the fractional Laplacian, setting up the notation for the rest of the thesis, while discussing the interest in it from a numerical analysis perspective.

The first fact that is important to mention, before starting to consider the problems of our interest, is that there are several definitions of the fractional Laplacian, that are equivalent on $\mathbb{R}^d$, and we refer to [129] for a complete review of them and proofs of their equivalence. However, when these definitions are restricted to bounded subsets of $\mathbb{R}^d$, incorporating boundary conditions, specific to the type of definition that is being used, they lead to different operators that generally fail to be equivalent with each other.

The work that will be presented has the aim of constructing numerical approximations for PDEs that involve the fractional Laplacian on a bounded region of space; therefore the choice of the definition of the fractional Laplacian is a crucial point for our studies. We will mainly use two definitions of the fractional Laplacian: for the evolutionary PDEs involving fractional operators, discussed in Chapters 1,2 and 3 we will adopt the spectral formulation of a fractional operator, while in Chapter 4 and 5 we propose a novel method for the fractional Laplacian in its integral definition. The reasons why different definitions are used depending on the problem will be made clear in the content of the thesis, but we anticipate that the spectral definition is well suited for the functional setting of the evolutionary PDEs, as it avoids some regularity complications that are associated with the integral definition. However, for the same reason, the integral definition is particularly interesting and challenging from a numerical perspective. Both of these definitions will be now presented in the main body of the introduction.

In order to illustrate to the reader the main ideas regarding the formulation of the fractional Laplacian and the intuition behind its nonlocal properties, we will first introduce the operator on $\mathbb{R}^d$ and illustrate its integral definition on it for its physical interpretation. We will then present the natural restriction of the integral fractional Laplacian to a bounded domain. Subsequently, we will introduce the spectral definition of the fractional Laplacian on a bounded domain. We will motivate the numerical challenges that both of these formulations present.

Let us denote by Δ the Laplace operator, called Laplacian. The Laplacian Δ on $\mathbb{R}^d$ is expressed as the divergence of the gradient,

$$\Delta = \nabla \cdot \nabla = \frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_d^2}.$$

The Laplace operator is a local operator, in the sense that the value of Δu at a point depends only on the values of u in an arbitrarily small neighbourhood of the point.

The Laplacian has a wide range of properties, among which there is its behaviour under the action of the Fourier transform. If we define the Fourier transform of a function $u : \mathbb{R}^d \rightarrow \mathbb{R}$ as

$$\mathcal{F}[u](\xi) = \hat{u}(\xi) := \int_{\mathbb{R}^d} u(x) e^{-2\pi i \xi \cdot x} dx,$$

we have that for a multi-index $\alpha = (\alpha_1, \dots, \alpha_d)$ the action of the Fourier transform is

$$\left(\frac{\partial}{\partial x} \right)^\alpha u(x) \xrightarrow{\mathcal{F}} (2\pi i)^{|\alpha|} \xi^\alpha \hat{u}(\xi),$$

where $|\alpha| := \alpha_1 + \dots + \alpha_d$, and therefore

$$(-\Delta)u(x) \xrightarrow{\mathcal{F}} (2\pi|\xi|)^2 \hat{u}(\xi). \quad (1)$$

Thus we can say that the Fourier transform pulls out a factor $(2\pi|\xi|)^2$ from the Laplacian.

A first way to introduce the fractional Laplacian on $\mathbb{R}^d$ is to ask whether the property (1) can be generalised to change the exponent in the power of the factor that we get out from the action of the Fourier transform. In other words, we can define the *fractional Laplacian* of a function $u : \mathbb{R}^d \rightarrow \mathbb{R}$ as the operator $(-\Delta)^s$ such that

$$(-\Delta)^s u \xrightarrow{\mathcal{F}} (2\pi|\xi|)^{2s} \hat{u},$$

for $0 < s < 1$. The exponent s is often called the *fractional order*. A first important remark is that the definition of the fractional Laplacian using the Fourier transform is a global definition, involving the whole of $\mathbb{R}^d$. This is an important difference with respect to the standard Laplacian.

We introduce now the integral definition or Riesz definition of the fractional Laplacian. This formulation provides an explicit expression for the fractional Laplacian, offering a physical interpretation of the intrinsic nonlocality of the operator. For these reasons, it is one of the most widely used definitions, but it presents both analytical and numerical challenges.

If we know the expression of the Fourier transform applied to a function, to reconstruct the function we can use the inverse Fourier transform, that is

$$u = \mathcal{F}^{-1}[\hat{u}](x) := \int_{\mathbb{R}^d} \hat{u}(\xi) e^{2\pi i x \cdot \xi} d\xi.$$

Thus, if we proceed formally, what we get is

$$\begin{aligned} (-\Delta)^s u(x) &= \mathcal{F}^{-1}[(2\pi|\xi|)^{2s} \mathcal{F}[u]](x) \\ &= (2\pi)^{2s} \int_{\mathbb{R}^d} |\xi|^{2s} \int_{\mathbb{R}^d} u(t) e^{-2\pi i \xi \cdot t} dt e^{2\pi i \xi \cdot x} d\xi. \end{aligned} \quad (2)$$

We can now take our formal procedure, namely expression (2), and through it provide an explicit representation of the fractional Laplacian. We start by recalling that for $-d < 2s < 0$ the term $|\xi|^{2s}$ admits the inverse Fourier transform given by

$$\mathcal{F}^{-1}[(2\pi|\xi|)^{2s}](x) = \frac{2^{2s} \Gamma(s + \frac{d}{2})}{\pi^{d/2} |\Gamma(-s)|} |x|^{-d-2s},$$

(see [166]), and the Fourier transform of a convolution of two functions is the product of their Fourier transforms,

$$f * g \xrightarrow{\mathcal{F}} \hat{f} \hat{g},$$

where the convolution of f and g on $\mathbb{R}^d$ is given by

$$(f * g)(x) := \int_{\mathbb{R}^d} f(x - y) g(y) dy.$$

If the fractional order was negative $-d/2 < s < 0$, calling $C_{d,s} := \frac{2^{2s}\Gamma(s+\frac{d}{2})}{\pi^{d/2}|\Gamma(-s)|}$, we could formally write an expression for (2),

$$(-\Delta)^s u(x) = C_{d,s} |x|^{-d-2s} * u(x) = C_{d,s} \int_{\mathbb{R}^d} u(y) \frac{1}{|x-y|^{d+2s}} dy. \quad (3)$$

As a matter of fact, the above expression can be extended for the case $s > 0$. The step needs mathematical care because for $s > 0$ the argument inside the integral renders the singularity at x nonintegrable; however, arguing by analytical continuation (see [131, p.45,46]), it is indeed possible to show that a similar expression is meaningful in the range $0 < s < 1$. More precisely, following [131], we can consider, for an arbitrary $\varphi \in C_0^\infty(\mathbb{R}^d)$, the expression

$$\psi(x, s) = (-\Delta)^s \varphi(x) = C_{d,s} \int_{\mathbb{R}^d} \varphi(x+z) \frac{1}{|z|^{d+2s}} dz,$$

which is an analytic function of s in the region $\operatorname{Re}(s) < 0$ with singular points $s = -\frac{d}{2} - n$, $n = 0, 1, \dots$. If one splits the expression, we have

$$\psi(x, s) = C_{d,s} \int_{\mathbb{R}^d \setminus B_1} \varphi(x+z) \frac{1}{|z|^{d+2s}} dz + C_{d,s} \int_{B_1} \frac{\varphi(x+z) - \varphi(x)}{|z|^{d+2s}} dz - \frac{C_{d,s}}{2s} \varphi(x) \omega_d,$$

where $B_1 = \{|z| < 1\}$ is the unit ball and $\omega_d = 2\pi^{d/2}/\Gamma(d/2)$ is the surface measure of the unit hypersphere in $\mathbb{R}^d$. The first and third terms in the expression above are regular for $\operatorname{Re}(s) > 0$ and for the second it is possible to show that

$$\int_{B_1} \frac{\varphi(x+z) - \varphi(x)}{|z|^{d+2s}} dz = \omega_d \int_0^1 (\tilde{\varphi}(x, r) - \varphi(x)) r^{-2s-1} dr,$$

where

$$\tilde{\varphi}(x, r) = \frac{1}{\omega_d} \int_{|y|=r} \varphi(x+y) d\omega_y,$$

where ω_y is the surface measure on the sphere $\{|y| = r\}$. Observing that $\tilde{\varphi}(x, r) - \varphi(x) = \mathcal{O}(r^2)$ as $r \rightarrow 0$ ([131, Pizzetti formula, p.46]), one concludes that the integral converges near the origin when $0 < s < 1$. Hence $\psi(x, s)$ extends analytically to $0 < \operatorname{Re}(s) < 1$. Finally, noting that within that strip it holds

$$-\frac{\omega_d}{2s} \varphi(x) = -\varphi(x) \int_{\mathbb{R}^d \setminus B_1} \frac{1}{|z|^{d+2s}} dz$$

it is possible to recombine the terms into a single expression in terms of $\int_{\mathbb{R}^d} (\varphi(x+z) - \varphi(x))/|z|^{d+2s} dz$.

With these considerations, the *integral fractional Laplacian* of a function $u : \mathbb{R}^d \rightarrow \mathbb{R}$ is then given by

$$\begin{aligned} (-\Delta)^s u(x) &= C_{d,s} \text{P.V.} \int_{\mathbb{R}^d} \frac{u(x) - u(y)}{|x-y|^{d+2s}} dy \\ &= C_{d,s} \lim_{\epsilon \rightarrow 0} \int_{\mathbb{R}^d \setminus B_\epsilon(x)} \frac{u(x) - u(y)}{|x-y|^{d+2s}} dy. \end{aligned} \quad (4)$$

The difference $u(x) - u(y)$ in the numerator, which vanishes at the singularity, provides a regularisation, which guarantees the existence of the principal value for smooth functions u with sufficient decay.

The expression (4) allows us to give a physical interpretation to the fractional Laplacian and highlight an analogy with the standard Laplacian. In fact, the Laplace operator can be seen as the measure of the infinitesimal displacement of a function, namely

$$\Delta u(x) \propto \lim_{r \rightarrow 0} \frac{1}{r^2 |B_r(x)|} \int_{B_r(x)} (u(y) - u(x)) dy,$$

(cf. [51] for further details) and if we look at (4) we can think of the fractional Laplacian as a weighted average of the oscillations of the function on $\mathbb{R}^d$, with weights given by the Riesz kernel $K_s(z) := C_{d,s} |z|^{-d-2s}$. While the averaging for the standard Laplacian takes place in a small neighbourhood of a point, the one for the fractional Laplacian involves the whole space. This highlights the nonlocal nature of the fractional Laplacian and shows that the fractional order s controls, in a way, the magnitude of the nonlocality, via the weight function in the average.

The definition (4) of the fractional Laplacian leads to the definition of the *fractional Sobolev-Slobodeckii spaces* of order $s \in (0, 1)$. If we denote the bilinear form

$$a_s(u, v) = \frac{C_{d,s}}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} \frac{(u(x) - u(y))(v(x) - v(y))}{|x - y|^{d+2s}} dx dy, \quad (5)$$

and the associated seminorm $|w|_{H^s(\mathbb{R}^d)} := a_s(w, w)^{1/2}$ accordingly, for $s \in (0, 1)$, we define

$$H^s(\mathbb{R}^d) := \left\{ w \in L^2(\mathbb{R}^d) \text{ such that } |w|_{H^s(\mathbb{R}^d)} < \infty \right\}, \quad (6)$$

endowed with the norm $\|w\|_{H^s(\mathbb{R}^d)}^2 := \|w\|_{L^2(\mathbb{R}^d)}^2 + |w|_{H^s(\mathbb{R}^d)}^2$. In our notation, the seminorm $\sqrt{2/C_{d,s}} \cdot |w|_{H^s(\mathbb{R}^d)}$ is called the *Gagliardo-Slobodeckii semi-norm*; the two seminorms are clearly equivalent (see [88, Proposition 3.6]).

For the fractional Laplacian on $\mathbb{R}^d$ we include a dutiful mention to the well-known Caffarelli–Silvestre extension [55], where the authors proved that any fractional power of the Laplacian can be determined as an operator that maps a Dirichlet boundary condition to a Neumann-type condition via an extension problem. More precisely, considering the function $\mathcal{U} = \mathcal{U}(x, y) : \mathbb{R}^d \times [0, \infty) \rightarrow \mathbb{R}$, solution of the extended problem

$$\begin{cases} \Delta_x \mathcal{U} + \frac{1-2s}{y} \partial_y \mathcal{U} + \partial_y^2 \mathcal{U} = 0, & x \in \mathbb{R}^d, y > 0, \\ \mathcal{U}(x, 0) = u(x), & x \in \mathbb{R}^d, \end{cases} \quad (7)$$

it holds

$$-\lim_{y \rightarrow 0_+} y^{1-2s} \partial_y \mathcal{U}(x, y) = C_s (-\Delta)^s u(x), \quad (8)$$

for a multiplicative constant C_s , depending only on s . This result still constitutes one of the great milestones in mathematical research on the fractional Laplacian, connecting the nonlocal

operator in $\mathbb{R}^d$ with a corresponding local elliptic problem, posed in $\mathbb{R}^{d+1}$. The extension method goes back to Molčanov and Ostrovskiĭ [144], in the context of symmetric stable processes, and was employed by other authors (e.g. [82]) before receiving a systematic treatment by Caffarelli and Silvestre.

In approaching evolutionary PDEs and their numerical analysis we have the need to confine the fractional Laplacian to functions that are defined on a bounded region of space in $\mathbb{R}^d$. The integral representation (4) can be used for functions defined only on a subset Ω of $\mathbb{R}^d$, however this must be done by choosing an adequate boundary condition, or more precisely a boundary condition that gives meaning to the values of u outside Ω . For example, one of the most natural choices for the fractional Laplacian in its integral representation is a Dirichlet boundary condition, which takes the form of an exterior condition imposing $u = 0$ on $\mathbb{R}^d \setminus \Omega$. As mentioned previously, it is precisely the choice of the boundary conditions that makes different definitions of the fractional Laplacian not equivalent on bounded domains.

From now on, when it is not specified differently we will denote by Ω a bounded open Lipschitz domain contained in $\mathbb{R}^d$. Additionally, we denote by n the outward unit normal to the boundary of the domain $\partial\Omega$ and we denote by ∂_n the (weak) directional derivative with respect to n . We denote by $(\cdot, \cdot)$ the $L^2(\Omega)$ inner product and by $\|\cdot\|_{L^p(\Omega)}$ and $\|\cdot\|_{H^1(\Omega)}$ the standard $L^p(\Omega)$ and $H^1(\Omega)$ norm, respectively. Let us also define the corresponding function spaces quotiented with the subspace of constant functions, which will be useful in the following; we will denote by $L_*^2(\Omega)$ and $H_*^1(\Omega)$ the closed linear subspace of $L^2(\Omega)$ and $H^1(\Omega)$ with zero integral average on Ω , respectively, that are,

$$\begin{aligned} L_*^2(\Omega) &:= \left\{ v \in L^2(\Omega) \text{ such that } \int_{\Omega} v \, dx = 0 \right\} \quad \text{and} \\ H_*^1(\Omega) &:= \left\{ v \in H^1(\Omega) \text{ such that } \int_{\Omega} v \, dx = 0 \right\}. \end{aligned}$$

With the integral definition of the fractional Laplacian, we can also introduce the fractional-order Sobolev space $H^s(\Omega)$ for $0 < s < 1$,

$$H^s(\Omega) := \left\{ u \in L^2(\Omega) \text{ such that } \int_{\Omega} \int_{\Omega} \frac{|u(x) - u(y)|^2}{|x - y|^{d+2s}} \, dx \, dy < \infty \right\},$$

and we endow it with the norm defined by

$$\|u\|_{H^s(\Omega)} := \left(\|u\|_{L^2(\Omega)}^2 + |u|_{H^s(\Omega)}^2 \right)^{\frac{1}{2}},$$

where the *Gagliardo–Slobodeckĭĭ semi-norm* $|\cdot|_{H^s(\Omega)}$ is given by

$$|u|_{H^s(\Omega)}^2 := \int_{\Omega} \int_{\Omega} \frac{|u(x) - u(y)|^2}{|x - y|^{d+2s}} \, dx \, dy.$$

This definition is in a way the natural analogue of the space (6) for a domain Ω . For $\sigma = m + s$, where m is a nonnegative integer and $s \in (0, 1)$, the Sobolev space of order $\sigma > 0$ is defined by

$$H^\sigma(\Omega) := \left\{ u \in H^m(\Omega) \text{ such that } \left(\frac{\partial}{\partial x} \right)^\alpha u \in H^s(\Omega) \text{ for all } \alpha \in \mathbb{N}^d, |\alpha| = m \right\},$$

where $H^m(\Omega)$ is the Sobolev space of order m and summability 2, $(\partial/\partial x)^\alpha$ stands for the weak derivative of multi-index $\alpha = (\alpha_1, \dots, \alpha_d)$ and order $|\alpha| := \alpha_1 + \dots + \alpha_d$, and $\mathbb{N}$ denotes the set of all nonnegative integers. Finally we also define the space $H_0^s(\Omega) := \overline{C_0^\infty(\Omega)}^{H^s}$.

We proceed now with the introduction of the spectral fractional Laplacian on a bounded domain and its related notations. Given the bounded domain Ω , consider

$$\mathcal{B}(\cdot) = 0 \quad \text{on} \quad \partial\Omega$$

as a homogeneous boundary condition. For example, with this notation, $\mathcal{B}(u) := u$ stands for a homogeneous Dirichlet boundary condition and $\mathcal{B}(u) := \partial_n u$ stands for a homogeneous Neumann boundary condition. Finally let V be a proper closed linear subspace of $H^1(\Omega)$, which depends on the boundary condition; for example $V := H_0^1(\Omega)$ if we are considering a Dirichlet boundary condition and $V := H_*^1(\Omega)$ if we are considering a Neumann boundary condition. In the case of a homogenous Dirichlet boundary condition we let $H^{-1}(\Omega)$ denote the dual space of $H_0^1(\Omega)$, whereas for a homogenous Neumann boundary condition $H^{-1}(\Omega)$ will denote the dual space of $H^1(\Omega)$; we then use $\langle \cdot, \cdot \rangle$ to refer to the associated duality pairing between $H^{-1}(\Omega)$ and $H_0^1(\Omega)$ or $H^1(\Omega)$, respectively. Analogously, in the case of a Dirichlet boundary condition we denote by $H^{-s}(\Omega)$ the dual space of the fractional-order Sobolev space $H_0^s(\Omega)$ for $\frac{1}{2} < s < 1$, while for a homogenous Neumann boundary condition we will denote by $H^{-s}(\Omega)$ the dual space of $H^s(\Omega)$ for $0 < s < 1$.

The pair $(\text{Dom}(-\Delta_{\mathcal{B}}), -\Delta_{\mathcal{B}})$ is defined as follows:

$$\begin{aligned} \text{Dom}(-\Delta_{\mathcal{B}}) := & \left\{ u \in V : V \ni v \mapsto \int_{\Omega} \nabla u \cdot \nabla v \, dx \right. \\ & \left. \text{is a continuous linear functional on } L^2(\Omega) \right\}, \\ \int_{\Omega} (-\Delta_{\mathcal{B}} u) v \, dx := & \int_{\Omega} \nabla u \cdot \nabla v \, dx, \quad u \in \text{Dom}(-\Delta_{\mathcal{B}}), v \in V. \end{aligned}$$

Thus, $-\Delta_{\mathcal{B}}$ is a nonnegative and self-adjoint linear operator that is densely defined in $L^2(\Omega)$ in the case of a Dirichlet boundary condition, and in $L_*^2(\Omega)$ in the case of the Neumann boundary condition; thanks to the Hilbert–Schmidt theorem (cf., for example, in [105, Lemma 5.1]), there exists an orthonormal basis of $L^2(\Omega)$, respectively $L_*^2(\Omega)$, consisting of eigenfunctions $\varphi_k \in V \setminus \{0\}$, $k = 1, 2, \dots$, with corresponding eigenvalues $0 < \lambda_1 \leq \lambda_2 \leq \dots \nearrow +\infty$. Thus, by writing $\mathcal{B}(\varphi_k) = \varphi_k$ if we have a Dirichlet boundary condition and $\mathcal{B}(\varphi_k) = \partial_n \varphi_k$ for a

Neumann boundary condition,

$$\begin{cases} -\Delta\varphi_k = \lambda_k\varphi_k & \text{in } \Omega, \\ \mathcal{B}(\varphi_k) = 0 & \text{on } \partial\Omega, \end{cases} \quad (9)$$

with the partial differential equation in the first line of (9) understood as an equality in $L^2(\Omega)$, and the homogeneous boundary condition appearing in the second line of (9) as an equality in $H^{\frac{1}{2}}(\partial\Omega)$ in the case of a Dirichlet boundary condition, and as an equality in $H^{-\frac{1}{2}}(\partial\Omega)$ in the case of a Neumann boundary condition. Let $-\Delta_{\mathcal{B}}$ denote the Laplacian associated with the boundary condition $\mathcal{B}$. For example $-\Delta_{\mathcal{B}}$ is the Dirichlet Laplacian, denoted as $-\Delta_D$, if $\mathcal{B}(u) := u$, or it is the Neumann Laplacian, denoted as $-\Delta_N$, if $\mathcal{B}(u) := \partial_n u$.

For $s \in (0, 1)$ the domain of the *spectral fractional Laplacian* $(-\Delta_{\mathcal{B}})^{s/2}$ is defined as the Hilbert space

$$\mathbb{H}_D^s(\Omega) := \left\{ u(\cdot) = \sum_{k=1}^{\infty} u_k \varphi_k(\cdot) \in L^2(\Omega) : \|u\|_{\mathbb{H}^s(\Omega)}^2 := \sum_{k=1}^{\infty} \lambda_k^s u_k^2 < \infty \right\}, \quad u_k := (u, \varphi_k) \quad (10)$$

for $k = 1, 2, \dots$ in the case of a homogeneous Dirichlet boundary condition, and

$$\mathbb{H}_N^s(\Omega) := \left\{ u(\cdot) = \sum_{k=1}^{\infty} u_k \varphi_k(\cdot) \in L_*^2(\Omega) : \|u\|_{\mathbb{H}^s(\Omega)}^2 := \sum_{k=1}^{\infty} \lambda_k^s u_k^2 < \infty \right\}, \quad u_k := (u, \varphi_k) \quad (11)$$

for $k = 1, 2, \dots$ if we are considering a homogeneous Neumann boundary condition. We use $\mathbb{H}^s(\Omega)$ as a unified notation for both of these cases; the distinction between them will be implicit in the type of Laplacian (i.e. Dirichlet or Neumann) that will be used and will be clear from the context. We denote by $\mathbb{H}^{-s}(\Omega)$ the corresponding dual space.

For $u \in \mathbb{H}^s(\Omega)$, we define the spectral fractional Laplacian by

$$(-\Delta_{\mathcal{B}})^s u(x) := \sum_{k=1}^{\infty} \lambda_k^s u_k \varphi_k(x), \quad (12)$$

as an element of $\mathbb{H}^{-s}(\Omega)$. Furthermore, one has $\|u\|_{\mathbb{H}^s(\Omega)} = \|(-\Delta_{\mathcal{B}})^{s/2} u\|_{L^2(\Omega)}$ for all $u \in \mathbb{H}^s(\Omega)$.

We stress further that the integral representation (4) and the spectral definition (12) fail to be equivalent on bounded domains Ω , once one has set the respective boundary conditions; in [164] the authors in fact show that with a Dirichlet boundary condition (that is given by setting $\mathcal{B}(u) = u$ for the spectral fractional Laplacian and by imposing $u = 0$ on $\mathbb{R}^d \setminus \Omega$ for the integral fractional Laplacian) the two operators have completely different spectra, highlighting their difference as operators.

The spectral fractional Laplacian on a bounded domain has additionally an explicit formula in terms of the heat semigroup of the Laplacian $(-\Delta_{\mathcal{B}})$ (cf., [167, eq. (1.11)])

$$(-\Delta_{\mathcal{B}})^s u(x) = \frac{1}{\Gamma(-s)} \int_0^{\infty} (e^{\tau \Delta_{\mathcal{B}}} u(x) - u(x)) \frac{1}{\tau^{1+s}} d\tau, \quad (13)$$

where $e^{\tau \Delta_{\mathcal{B}}} u(x)$ is the solution of the heat equation

$$\begin{cases} \frac{\partial w}{\partial \tau} = \Delta w & \text{in } \Omega \times (0, \infty), \\ w(x, 0) = u(x) & \text{in } \Omega, \\ \mathcal{B}(w(x, \tau)) = 0 & \text{on } \partial\Omega \times [0, \infty). \end{cases} \quad (14)$$

This formulation of the spectral fractional Laplacian allows for a stochastic interpretation of the operator. In fact, the probabilistic setting related to the spectral fractional Laplacian is more sophisticated and we refer to [91, 92] for a detailed and rigorous description of it for a Dirichlet and a Neumann boundary condition, respectively. The authors show that the spectral fractional Laplacian is the generator of a so-called subordinate Brownian motion, determined by a time-weighted superposition of the classical heat kernel, the weights being the law of a random clock. Loosely speaking, the stochastic process generated by the spectral fractional Laplacian takes a Brownian motion on a bounded domain, subject to a given boundary condition and runs it along a random clock: for a particle in this process, when the clock leaps, the particle reappears at the endpoint of a Brownian excursion run at fast-forward, so that the apparent jump conceals a continuous path, and that path must obey the imposed boundary condition. This way of thinking of the spectral fractional Laplacian further motivates the advantage of having a natural way to encode different sorts of boundary conditions into the setting of the operator, preserving the nonlocality of the jump process.

Finally, we mention that the operator (12) also admits a Caffarelli-Silvestre type extension, that we include for completeness, referring to [57, 167]. Let $U = U(x, y) : \Omega \times [0, \infty) \rightarrow \mathbb{R}$ be the solution to the following extension problem

$$\begin{cases} \Delta_x U + \frac{1-2s}{y} \partial_y U + \partial_y^2 U = 0 & \text{in } \Omega \times (0, \infty), \\ \mathcal{B}(U(x, y)) = 0 & \text{on } \partial\Omega \times [0, \infty), \\ U(x, 0) = u(x) & \text{on } \Omega. \end{cases} \quad (15)$$

Then

$$-\frac{1}{2s} \lim_{y \rightarrow 0^+} y^{1-2s} U_y(x, y) = \frac{|\Gamma(-s)|}{4^s \Gamma(s)} (-\Delta_{\mathcal{B}})^s u(x). \quad (16)$$

Once one has given meaning to the fractional Laplacian $(-\Delta)^s$ the interest moves rapidly to equations involving the fractional Laplacian and, from a numerical perspective, to the computation of their solutions. The first problem that has been at the centre of a large part of mathematical research about the fractional Laplacian is the simple, yet challenging, fractional counterpart of the Poisson equation, that is what we call the *fractional Poisson equation*: given a function f find the solution u to

$$(-\Delta)^s u = f. \quad (17)$$

This elliptic problem by itself has been an inexhaustible source for research in analysis, offering several directions for research (e.g. regularity of u , dependence on the type of bounded domain, behaviour of u at the boundary).

For the purpose of additionally motivating the difference between the two operators (4) and (12) on a bounded domain, there is a qualitative difference of the solutions to (17) with a Dirichlet boundary condition, that is worth mentioning at this stage: using (4) with $u = 0$ on $\mathbb{R}^d \setminus \Omega$, for any $s \in (0, 1)$ the solution u behaves like d_Ω^s in a neighbourhood of the boundary $\partial\Omega$, where $d_\Omega(x) = \text{dist}(x, \mathbb{R}^d \setminus \Omega)$ (see [1] and [104, Section 2.7]), while using (12) with $\mathcal{B}(u) = u$, the solution u exhibits a different regularity, behaving simply as d_Ω for $s > 1/2$ and as d_Ω^{2s} for $s \leq 1/2$ (see [57]). This observation concerning the difference in regularity of the solution of the fractional Poisson equation will be at the centre of the work of Chapter 4.

Alongside the study of elliptic problems as (17), over the past two decades work has also been devoted to evolutionary PDEs involving the fractional Laplacian. A broad and diverse body of literature has emerged, in which the fractional Laplacian is used to model nonlocal diffusion, as well as reactions, interactions, and other time-dependent effects. Here we ought to mention the fractional heat equation

$$\frac{\partial u}{\partial t} = -(-\Delta)^s u, \quad (18)$$

as an example of an evolutionary problem widely used in applications to model long-jump diffusion, and as the simplest prototype of a parabolic equation involving the fractional Laplacian. The fractional heat equation has been studied in a large number of papers, mainly coming from probability, but from a modern PDE perspective, early work on equations like (18) with more general nonlocal operators can be found in [54, 103] and subsequently [26, 37] developed a theory of existence, uniqueness and regularity of solutions for it. We mention also the works [80, 81, 172] where more general nonlinear fractional diffusion equations of the form

$$\frac{\partial u}{\partial t} = -(-\Delta)^s \varphi(u), \quad (19)$$

were studied, including the porous-medium-type case $\varphi(u) = |u|^{m-1}u$, $m > 0$; we refer the reader to [170] for a survey on these types of problems.

As a matter of fact, a large part of the work that we present in the thesis will be devoted to the (numerical) analysis of evolutionary equations that involve the fractional Laplacian.

From a numerical perspective the main question arising from (17) and related time-dependent problems is how to provide an accurate and efficient algorithm to approximate $(-\Delta)^s$ and hence compute u in (17) on bounded domains. The numerical approximation of $(-\Delta)^s$ clearly depends on the definition chosen for the fractional Laplacian.

The definition (4) is fundamental and widely used because it is an explicit expression for the fractional Laplacian, based on which one can directly design numerical schemes. In fact, for the integral formula a variety of methods have been proposed through the years.

Finite difference schemes approximate the principal-value integral by discretising the associated singular convolution; these methods are simple to construct and are widely used on regular meshes over axiparallel domains, but are difficult to adopt in different cases. In [124] the authors proposed finite difference methods for fractional diffusion equations, demonstrating robust convergence for smooth solutions. The authors of [84, 86] analysed and developed further finite difference methods for differential equations involving the fractional Laplacian and in [83] a similar finite difference scheme is used for more general fractional-order differential operators. We also refer to [95] for a finite difference discretization of the fractional Laplacian that is presented both in two and three dimensions and then applied to a fractional Allen–Cahn equation. These techniques benefit from their conceptual simplicity and ease of implementation, but they also have disadvantages, including limited flexibility on nonuniform grids and irregular domain geometries.

In the context of the integral representation (4), a finite element method provides a powerful variational framework. Through the use of suitable weak formulations, these techniques deliver accurate numerical solutions, particularly for irregular domains or problems whose solutions exhibit singular behaviour near domain boundaries. These methods have been developed to handle singularities in the kernel, adaptive refinement of the computational mesh, and incorporate efficient quadrature schemes for numerical integration. In the pioneering work [5] the authors introduced a piecewise linear conforming FEM for the integral fractional Laplacian, focusing on accurate truncation and error control. Subsequently, adaptive quadrature rules for finite element discretizations were developed in [6], ensuring efficient computation in irregular geometries. We refer also to [46, 47] for a discussion on local error estimates and the use of graded meshes. In [42] the authors developed a nonconforming finite element scheme, based on a sinc quadrature scheme to approximate the integral representation and discussed consistency of their method in approximating the bilinear form (5). These techniques retain all the advantages of a FEM, however, because they rely on the integral representation of the fractional Laplacian, they still face issues related to their high computational and implementation complexity due to dense matrix representations and numerical integration; for example adaptive mesh refinement is often needed to address the singularity of the kernel.

Several approaches in the literature have proposed numerical methods for the spectral fractional Laplacian. From a finite element perspective, [43], with subsequent developments discussed in [44, 39] proposed a scheme for the approximation of the spectral fractional Laplacian, without computing explicitly fractional powers A^s of the matrix representation A of the discrete Laplacian, but passing through an integral representation and designing a proper quadrature rule for it; this method was then applied in [40, 41] for fractional parabolic problems as the fractional heat equation. The works [77, 76] used explicit representations of the spectral fractional Laplacian involving the heat semigroup (13), combining suitable quadrature formulae of the

integral with a finite element method for the approximation of the solution of the corresponding heat equation.

Finite element methods have also been developed for the extension problem (15); they were first introduced in the work [146] that developed a FEM, providing rigorous error analysis and convergence rates. The method had the disadvantage of requiring additional computational resources to solve a PDE in higher dimensions, as well as a sufficiently refined graded mesh. Some of these issues were subsequently addressed in the innovative work [17] and the subsequent contribution [18]: following the observations of [146] on the analytical regularity in the extended dimension, the authors proved for the first time exponential convergence using an *hp*-FEM. Previously, *hp*-finite elements for the fractional Laplacian had been also used in [142] and after several contributions have continued to navigate the field; notable mentions in the topic, including a recent implementation of *hp*-FEM, are [19, 101, 12, 13] and [143], where *hp*-FEM is applied to a fractional heat equation.

For a recent survey on numerical methods for the fractional Laplacian and fractional diffusion we refer the reader to [38].

The thesis is structured in five chapters. Chapter 1 is focused on a finite element method for a nonlinear and nonlocal porous medium equation with a fractional pressure, obtained via the use of the fractional Laplacian. The equation makes use of the fractional Laplacian in its spectral definition (12) on a bounded domain and we rigorously prove convergence of the sequence of finite element approximations defined by the numerical scheme. The proof of convergence in Chapter 1 can be viewed both as the first rigorous finite element scheme for this type of nonlocal porous medium equation and also as a constructive argument for the proof of existence of solutions on a bounded domain using the spectral definition of the fractional Laplacian. Chapter 2 concerns the computational aspects of the FE scheme for the equation studied in Chapter 1, with a focus on the efficient computation of the FE approximation of the fractional Laplacian in its spectral definition using the theory of rational approximations. Chapter 2 contains a variety of simulations and numerical experiments validating the accuracy of the algorithms and some of the properties of the fractional porous medium equation and a related problem, that is the fractional Keller–Segel equation, for which we provide the first numerical investigation of the conditions under which blow-up of the solution occurs. Chapter 3 generalises the numerical method of Chapter 1 to a new and broader class of PDEs modelling nonlocal diffusion of porous medium type in the presence of anisotropy and confinement potentials. In the end, Chapters 4 and 5 move from evolutionary PDEs involving the spectral definition of the fractional Laplacian to an elliptic problem with the fractional Laplacian in its integral form (4). In this context, we propose a novel method for the fractional Dirichlet problem that addresses the lack of regularity of the solution of (17), that we have previously mentioned, and improves the error estimates that are available in the literature under regularity assumptions on the domain. We also discuss the

approximation and the implementation of the bilinear form (5), necessary to compute solutions in practice.

The thesis presents novel approaches and numerical methods for the fractional Laplacian from different perspectives. The development of techniques and algorithms for different problems with different definitions of the fractional Laplacian is meant to showcase a variety of effective methodologies and, at the same time, to open new directions for future work on the topic.

Chapter 1 is based on [62], published in *Numerische Mathematik*. Chapter 2 is based on the preprint [65], under review. Chapter 3 is based on the preprint [108], currently under review. Chapter 4 is based on the preprint [85], to be submitted. Chapter 5 will be made available as a preprint in the near future and submitted to a *Scientific Computing* journal.

You should have sat through some of those nights of argument and discussion. The questions, the inspection, oh, the lovely thinking – the beautiful thinking.

John Steinbeck (1902-1968), “East of Eden”

1

Finite element approximation of the fractional porous medium equation

1.1 The fractional porous medium model

We now introduce the type of evolutionary PDE problem that we are going to study. Our principal aim is to construct and analyse a numerical scheme for a porous medium equation involving the fractional Laplacian and other related models and generalisations.

In addition to the need of working on a bounded domain, we shall have to consider a specific boundary condition associated with the domain, that for our type of problems will be mainly a Neumann boundary condition. Such a condition will ensure conservation of mass of the solution, which is a relevant property that we aim to preserve. The imposition of this type of boundary condition with the use of the integral representation (4) would add several numerical difficulties. For this reason we will use the spectral definition (12) of the fractional Laplacian on a bounded domain; even though it lacks a physical interpretation, compared to the explicit representation (4), it will be seen to be mathematically convenient in the analysis of our finite element scheme.

Let us denote by ρ a certain density distribution and by $\mathbf{v}$ a velocity field; both are functions of space and time, $\rho = \rho(x, t)$, $\mathbf{v} = \mathbf{v}(x, t)$, the velocity is a vector function and we assume the density to be nonnegative, $\rho(x, t) \geq 0$. We relate the density and the velocity field via the continuity equation

$$\frac{\partial \rho}{\partial t} - \nabla \cdot (\rho \mathbf{v}) = 0. \quad (1.1a)$$

We postulate that the velocity $\mathbf{v}$ derives from a potential $c = c(x, t)$ through the equality

$$\mathbf{v} = -\nabla c. \quad (1.1b)$$

This happens for instance when ρ is the density of a fluid whose motion is modelled by Darcy's law, which relates velocity and pressure of the fluid (in that case c denotes the pressure). The potential can then be related in a closed form to the density $c = c(\rho)$ through a suitable equation of state, leading to various different models. For example, the simplest case $c = 2k\rho$ in fluid flow modeling, with k signifying a positive constant, pertains to filtration of a fluid through a porous stratum in the isothermal setting; this is the standard model for groundwater infiltration, Boussinesq's equation $\rho_t = k \Delta \rho^2$ (see [27]). More generally one has the nonlinear model $\rho_t = k \Delta \rho^m$ for $m > 1$.

The structure of the porous medium can be very complex, however: different pores, tubes and water filaments can make the phenomenon difficult to study, and standard models fail in accurately describing these complex features. A number of experimentalists have shown that in certain porous media, such as construction materials, classical diffusion cannot accurately predict the evolution of moisture. It was observed in particular that the wetting front may move in a significantly different way than classical models predict; for instance, in [161] the authors discuss solute transport in aquifers and they explain that standard dispersion can only occur in homogeneous aquifers. To address this issue, different models have been proposed in which nonlocal interactions and effects are present. For example, in [162] the authors propose a porous medium modelled with a network of channels of all length-scales through which the water particles can move over a very long distance.

As we discussed in the Introduction, the mathematical tool that we adopt in order to introduce nonlocal effects is the fractional Laplacian $(-\Delta)^s$, $s \in (0, 1)$. As the object of our study, we will then consider a nonlocal porous medium equation, in which the long-range interactions are modelled by a fractional-order elliptic equation; more precisely, we will consider

$$-(-\Delta)^s c = \rho, \quad 0 < s < 1. \quad (1.1c)$$

If $s = 0$ we recover the standard porous medium equation, while the case $s = 1$ has been investigated in [138, 70, 97].

The model (1.1) has been justified in the hydrological setting in [148], where a deterministic derivation of the equation was presented, subject to the assumption that the fluid in the porous medium can contribute to the flux at any point with long jumps depending only on the distance. The system (1.1) also arises in other contexts: a model similar to the case $s = 1$ was considered in [8] to describe the evolution of vortex-density in superconductors, while the equation with $s = \frac{1}{2}$ was suggested in [122] to model the motion of dislocations in a continuum. These equations also find applications in modelling charged particle transport in materials, since they are fractional counterparts of classical drift-diffusion equations for semiconductors [138]. For further discussion concerning models of porous medium diffusion with a nonlocal pressure of this type we refer to [171, Section 5.6.1], where it is noted that the problem in a bounded domain with Dirichlet or

Neumann boundary conditions has not been studied and computational techniques to deal with these kinds of nonlocal effects and the design of generic numerical schemes for this model are needed.

Instead of the first-order hyperbolic equation (1.1) we will consider a parabolic regularisation of the problem, where standard Fickian diffusion is present with the positive diffusion coefficient scaled to 1, because its specific value is of no relevance to the discussion herein. This leads to the following system:

$$\begin{cases} \frac{\partial \rho}{\partial t} = \Delta \rho - \nabla \cdot (\rho \nabla c), \\ -(-\Delta)^s c = \rho. \end{cases} \quad (1.2)$$

The fractional porous medium equation on $\mathbb{R}^d$ is obtained by inverting the fractional operator $(-\Delta)^s$ in terms of its fundamental solution U_s , i.e., $-c = U_s * \rho$, and plugging this into the first equation in (1.2), which then yields

$$\frac{\partial \rho}{\partial t} = \Delta \rho + \nabla \cdot (\rho \nabla (U_s * \rho)). \quad (1.3)$$

The previous equation has formally the structure of a Wasserstein gradient flow of an energy functional $\mathcal{E}(\rho)$, as in [63, 7, 64] for instance, if mass is normalized, thanks to it being conserved. Consequently, it leads to an evolution of densities governed by the dissipation of the free energy functional

$$\mathcal{E}(\rho) := \int_{\mathbb{R}^d} \rho \log \rho \, dx + \frac{1}{2} \int_{\mathbb{R}^d} (U_s * \rho) \rho \, dx,$$

where the first term is the Boltzmann entropy and the second term is the total interaction potential energy.

It has been shown in [60, 56, 71] that under suitable assumptions there exists a weak solution to (1.1) and (1.2) on the whole of $\mathbb{R}^d$, which has several properties, including conservation of mass, the dissipation of the free energy functional, and the decay of the spatial L^∞ norm in time. We will show that our numerical scheme has some of these features as well. Moreover in the recent works [59, 67] the asymptotic behaviour of solutions to (1.1) has been investigated where the dissipation of the free energy functional plays a key role. The existence of a smooth solution on $\mathbb{R}^d$ to the equation (1.2) or equivalently (1.3), supplemented with an initial condition, has been proved in [73]. Indeed, a large portion of the available literature for this type of equation considers the model on the whole of $\mathbb{R}^d$ written in the form (1.3) as it uses the integral definition of the fractional Laplacian (4); see [51] for further details.

We shall supplement the partial differential equations (1.2) with an initial condition for ρ and boundary conditions for ρ and c ; as we mentioned, the most natural choice for the latter are no-flux boundary conditions for both ρ and c . Let $\Omega \subset \mathbb{R}^d$ be a bounded open Lipschitz domain and additionally convex, simply for ease of triangulating Ω , we shall confine ourselves to the case when Ω is a convex polytopal Lipschitz domain in $\mathbb{R}^d$, $d = 2, 3$. Thus the initial-boundary-value problem we shall be considering is the following:

$$\begin{cases} \frac{\partial \rho}{\partial t} = \Delta \rho - \nabla \cdot (\rho \nabla c) & \text{in } \Omega \times (0, \infty), \\ -(-\Delta_N)^s c = \rho^* & \text{in } \Omega \times (0, \infty), \\ \partial_n \rho = 0, \quad \partial_n c = 0 & \text{on } \partial\Omega \times (0, \infty), \\ \rho(x, 0) = \rho_0(x) & \text{for all } x \in \Omega, \end{cases} \quad (1.4)$$

where $\rho_0 \in L^\infty(\Omega)$ is a given nonnegative initial datum, with normalized mass $\frac{1}{|\Omega|} \int_\Omega \rho_0 \, dx = 1$, the fractional Neumann Laplacian $(-\Delta_N)^s$ is understood to be based on its spectral definition (12), that we recall to be

$$(-\Delta_N)^s u(x) := \sum_{k=1}^{\infty} \lambda_k^s u_k \varphi_k(x), \quad (1.5)$$

for $u \in \mathbb{H}^s(\Omega)$. Finally ρ^* stands for the projection of ρ into the space of functions with zero integral average, namely

$$\rho^* := \rho - \bar{\rho}, \quad \text{with } \bar{\rho} := \frac{1}{|\Omega|} \int_\Omega \rho \, dx. \quad (1.6)$$

We note that the boundary condition $\partial_n c = 0$, explicitly stated for completeness, is already implicit in the use of the Neumann Laplacian $-\Delta_N$.

Having stated the problem (1.4) we now propose its weak formulation. Let $V := H^1(\Omega)$. The weak formulation of the initial-boundary-value problem (1.4) is as follows:

$$\begin{aligned} & \text{Find } \rho \in L^2(0, T; V) \text{ with } \frac{\partial \rho}{\partial t} \in L^2(0, T; V') \text{ such that} \\ & \left\langle \frac{\partial \rho}{\partial t}, \phi \right\rangle = - \int_\Omega \nabla \rho \cdot \nabla \phi \, dx + \int_\Omega \rho \nabla c \cdot \nabla \phi \, dx \quad \text{for all } \phi \in V \text{ and a.e. } t \in (0, T], \end{aligned} \quad (1.7a)$$

subject to the initial condition $\rho(x, 0) = \rho_0(x)$, where $\rho_0 \in L^\infty(\Omega)$ and $\rho_0(x) \geq 0$ for a.e. $x \in \Omega$ and where

$$-(-\Delta_N)^s c = \rho^* \text{ in } \Omega, \quad (1.7b)$$

with ρ^* given by (1.6). Notice that c is well defined, as the solution to the fractional equation (1.7b) exists and it is unique by Theorem A.1; we will therefore write $c = -(-\Delta_N)^{-s} \rho^*$, where $(-\Delta_N)^{-s}$ stands for the inverse of the spectral fractional Neumann Laplacian (1.5). When we speak of a weak solution to the problem (1.7) we mean a couple ρ and c such that (1.7a) and (1.7b) hold.

Now let us assume that a weak solution to problem (1.7) exists and that ρ is nonnegative almost everywhere in $\Omega \times [0, T]$. The existence of a weak solution to our problem and its nonnegativity will be rigorously proved in the next sections. In order to motivate the argument which our proof is based upon, we shall now perform preliminary formal computations; in these formal computations we shall additionally assume that the functions ρ and c have all the regularity that we need in order to ensure that our calculations are meaningful.

The first remark we make is that, if we take $\phi \equiv 1$ as test function in the weak formulation (1.7), then we have conservation of mass, in the sense that $\frac{1}{|\Omega|} \int_\Omega \rho(x, t) \, dx = \frac{1}{|\Omega|} \int_\Omega \rho(x, 0) \, dx =$

$\frac{1}{|\Omega|} \int_{\Omega} \rho_0(x) dx = 1$ for all $t \geq 0$, and because $\rho(x, t)$ is assumed to be nonnegative for all $t \geq 0$, also

$$\|\rho(t)\|_{L^1(\Omega)} = \|\rho_0\|_{L^1(\Omega)} \quad \text{for } t \geq 0.$$

A further important property that holds true for our equation is that $\|\rho(t)\|_{L^\infty(\Omega)} \leq \|\rho_0\|_{L^\infty(\Omega)}$. This fact is shown in [71] for the integral definition of the fractional Laplacian on $\mathbb{R}^d$. We will follow a similar strategy for our argument and show that the property holds true when Ω is a bounded Lipschitz domain, and using the spectral definition of the fractional Neumann Laplacian. We will also show later on that a similar statement holds true for a discretization of our problem.

Lemma 1.1. *Let ρ be a nonnegative smooth solution of the initial-boundary-value problem (1.4), let $F \in C^2([0, \infty))$ be a convex function, and suppose that $F(\rho_0) \in L^1(\Omega)$. Then,*

$$\frac{d}{dt} \int_{\Omega} F(\rho) dx \leq 0.$$

Proof. Assume first that F'' is bounded. Then, $F'(\rho) - F'(0)$ with $\rho \in H^1(\Omega)$ is an admissible test function in the weak formulation (1.7a). Thus we additionally have that

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} F(\rho) dx &= - \int_{\Omega} \nabla \rho \cdot \nabla F'(\rho) dx - \int_{\Omega} \rho F''(\rho) \nabla \rho \cdot \nabla (-\Delta_N)^{-s} \rho^* dx \\ \Leftrightarrow \frac{d}{dt} \int_{\Omega} F(\rho) dx &= - \int_{\Omega} F''(\rho) |\nabla \rho|^2 dx - \int_{\Omega} \rho F''(\rho) \nabla \rho \cdot \nabla (-\Delta_N)^{-s} \rho^* dx \\ \Leftrightarrow \frac{d}{dt} \int_{\Omega} F(\rho) dx &= - \underbrace{\int_{\Omega} F''(\rho) |\nabla \rho|^2 dx}_{\textcircled{1}} - \underbrace{\int_{\Omega} H(\rho) (-\Delta_N)^{1-s} \rho^* dx}_{\textcircled{2}}, \end{aligned} \quad (1.8)$$

where $H(r) := \int_0^r t F''(t) dt$. Notice that H is a nondecreasing function by definition.

Term $\textcircled{1}$ is clearly nonnegative. For term $\textcircled{2}$ we notice that letting $1 - s = \frac{\alpha}{2}$ we can use the explicit representation of the spectral fractional Laplacian, given by (13).

We note that by the definition (1.6) of ρ^* we have that $e^{\tau \Delta_N} \rho^* = e^{\tau \Delta_N} \rho - \bar{\rho}$. Thus,

$$\begin{aligned} \textcircled{2} &= \int_{\Omega} H(\rho(x)) \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty (e^{\tau \Delta_N} \rho^*(x) - \rho^*(x)) \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau dx \\ &= \int_{\Omega} H(\rho(x)) \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty (e^{\tau \Delta_N} \rho(x) - \rho(x)) \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau dx \\ &= \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty \left(\int_{\Omega} H(\rho(x)) e^{\tau \Delta_N} \rho(x) dx - \int_{\Omega} H(\rho(x)) \rho(x) dx \right) \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau \\ &= \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty ((e^{\tau \Delta_N} \rho, H(\rho)) - (\rho, H(\rho))) \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau. \end{aligned}$$

Let $W_\tau(x, y)$ be the distributional heat kernel for $-\Delta$ subject to a homogeneous Neumann boundary condition and $\tau > 0$. We have that $W_\tau \geq 0$ for all $\tau > 0$ and, for $u, v \in L^2(\Omega)$,

$$(e^{\tau \Delta_N} u, v) = \int_{\Omega} \int_{\Omega} W_\tau(x, y) u(y) v(x) dy dx.$$

Therefore, by plugging the heat kernel in the expression above, we deduce that

$$\begin{aligned}
\textcircled{2} &= \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty \int_\Omega \left(\int_\Omega W_\tau(x, y) \rho(x) H(\rho(y)) dx - \rho(y) H(\rho(y)) \right) dy \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau \\
&= \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty \int_\Omega \left(\int_\Omega W_\tau(x, y) (\rho(x) - \rho(y)) H(\rho(y)) dx \right. \\
&\quad \left. + \rho(y) H(\rho(y)) \left(\int_\Omega W_\tau(x, y) dx - 1 \right) \right) dy \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau \\
&= \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty \int_\Omega \int_\Omega W_\tau(x, y) (\rho(x) - \rho(y)) H(\rho(y)) dy dx \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau \\
&\quad + \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty \int_\Omega \rho(y) H(\rho(y)) (e^{\tau \Delta_N} 1(y) - 1) dy \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau.
\end{aligned}$$

By exchanging x and y and using the symmetry of the heat kernel we have also

$$\begin{aligned}
\textcircled{2} &= - \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty \int_\Omega \int_\Omega W_\tau(x, y) (\rho(x) - \rho(y)) H(\rho(x)) dy dx \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau \\
&\quad + \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty \int_\Omega \rho(y) H(\rho(y)) (e^{\tau \Delta_N} 1(y) - 1) dy \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau.
\end{aligned}$$

By summing the two expressions for $\textcircled{2}$ we then find that

$$\begin{aligned}
\textcircled{2} &= - \frac{1}{2\Gamma(-\alpha/2)} \left(\int_0^\infty \int_\Omega \int_\Omega W_\tau(x, y) (\rho(x) - \rho(y)) (H(\rho(x)) - H(\rho(y))) dx dy \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau \right. \\
&\quad \left. + 2 \int_0^\infty \int_\Omega \rho(y) H(\rho(y)) (1 - e^{\tau \Delta_N} 1(y)) dy \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau \right).
\end{aligned}$$

Thanks to the definition of $e^{\tau \Delta_N}$ stated in (14) we have that $e^{\tau \Delta_N} 1(y) \equiv 1$, which results in a convenient simplification of the expression for term $\textcircled{2}$ appearing in the last equality. Hence, from the monotonicity of H and the fact that $\Gamma(-\alpha/2) < 0$ we finally deduce that $\textcircled{2} \geq 0$. In the general case (i.e., when F'' is not bounded) we define $F_k(u) := F(0) + F'(0)u + \int_0^u \int_0^v \min(F''(w), k) dw dv$ for $k > 0$; then, $F_k''(u)$ is bounded and the result follows for F replaced by F_k and taking the limit $k \rightarrow \infty$ using monotone convergence. $\square$

The previous result allows us to prove the following lemma, which provides a bound on the $L^\infty(\Omega)$ norm of $\rho(t)$ in terms of $\|\rho_0\|_{L^\infty(\Omega)}$.

Lemma 1.2. *Let ρ be a nonnegative smooth solution of the initial-boundary-value problem (1.4). The following inequality holds for all $t \geq 0$:*

$$\|\rho(t)\|_{L^\infty(\Omega)} \leq \|\rho_0\|_{L^\infty(\Omega)}.$$

Proof. By the previous lemma we have that

$$\sup_{t>0} \int_\Omega F(\rho(t)) dx \leq \int_\Omega F(\rho_0) dx.$$

We choose a nonnegative convex function $F \in C^2([0, \infty))$ such that $F(u) = 0$ for $u \leq \|\rho_0\|_{L^\infty(\Omega)}$ and $F(u) > 0$ for $u > \|\rho_0\|_{L^\infty(\Omega)}$. Then,

$$0 \leq \int_{\Omega} F(\rho(t)) \, dx \leq \int_{\Omega} F(\rho_0) \, dx = 0 \quad \text{for } t \geq 0,$$

and thus $0 \leq \rho(x, t) \leq \|\rho_0\|_{L^\infty(\Omega)}$ for $t \geq 0$. $\square$

Lemma 1.2 together with the nonnegativity of ρ and mass conservation implies that $\|\rho(t)\|_{L^p(\Omega)}$ is bounded for all $t \geq 0$ and $1 \leq p \leq \infty$.

We continue by investigating the energy structure of our problem (1.7). Let us define the nonnegative convex function $G \in C([0, \infty))$ by

$$G(r) := r(\log r - 1) + 1 \quad \text{for } r > 0 \quad \text{and} \quad G(0) := 1. \quad (1.9)$$

We note that $G(1) = 0$ and $\lim_{r \rightarrow +\infty} G(r)/r = +\infty$. We shall assume for the moment that $\rho(x, t) \geq 0$ for all $x \in \Omega$ and all $t > 0$ and its spatial integral is normalized as $\frac{1}{|\Omega|} \int_{\Omega} \rho(x, t) \, dx = 1$, and consider, as discussed in the Introduction, the free energy functional

$$E(\rho) := \int_{\Omega} G(\rho) \, dx - \frac{1}{2} \int_{\Omega} c \rho \, dx = \int_{\Omega} G(\rho) \, dx - \frac{1}{2} \int_{\Omega} c \rho^* \, dx, \quad (1.10)$$

where the second equality follows thanks to the fact that c has zero integral average on Ω (cf. Theorem A.1). Both terms appearing in the free energy functional (1.10) are nonnegative. Indeed, by applying Jensen's inequality with the uniform probability measure $d\mu(x) := \frac{1}{|\Omega|} dx$ on Ω to the convex function G yields that

$$\int_{\Omega} G(\rho) \, d\mu(x) \geq G\left(\int_{\Omega} \rho(x) \, d\mu(x)\right) = 0,$$

thanks to the normalization of ρ and the conservation of mass. On the other hand, we can express the second term in (1.10) in terms of the eigenvalues and eigenfunctions of the Neumann Laplacian as follows:

$$-\frac{1}{2} \int_{\Omega} c \rho^* \, dx = \frac{1}{2} \sum_{k=1}^{\infty} \lambda_k^s c_k^2 \geq 0,$$

using that $-(-\Delta_N)^s c = \rho^*$ on Ω , in conjunction with the definition (1.5) of the fractional Neumann Laplacian and Parseval's identity in $L_*^2(\Omega)$. Therefore, the free energy functional $E(\rho)$ is a suitable quantity for controlling the 'distance' between ρ and μ , the uniform density on the domain Ω ; this will be rigorously proved in Theorem 1.23 stated in Section 1.3.

Lemma 1.3. *Let ρ be a nonnegative smooth solution of the initial-boundary-value problem (1.4). The following free energy identity holds for all $t \geq 0$:*

$$\frac{d}{dt} E(\rho) = - \int_{\Omega} \rho |\nabla(\log \rho - c)|^2 \, dx \leq 0. \quad (1.11)$$

Proof. By (formally) differentiating $E(\rho)$ with respect to t we have

$$\frac{d}{dt}E(\rho) = \int_{\Omega} \rho_t G'(\rho) dx - \frac{1}{2} \int_{\Omega} c_t \rho^* dx - \frac{1}{2} \int_{\Omega} c \rho_t dx.$$

Recalling that we have conservation of mass, $\frac{d}{dt} \int_{\Omega} \rho dx = 0$, and so $\partial_t \rho^* = \partial_t \rho$, it follows that

$$\int_{\Omega} c_t \rho^* dx = - \int_{\Omega} ((-\Delta_N)^{-s} \rho_t^*) \rho^* dx = - \int_{\Omega} \rho_t (-\Delta_N)^{-s} \rho^* dx = \int_{\Omega} \rho_t c dx,$$

by the fact that $-\Delta_N$ is self-adjoint. As a consequence, using the weak formulation (1.7a), we have

$$\begin{aligned} \frac{d}{dt}E(\rho) &= \int_{\Omega} \rho_t \log \rho dx - \int_{\Omega} \rho_t c dx = \int_{\Omega} \rho_t (\log \rho - c) dx \\ &= - \int_{\Omega} \rho \nabla \log \rho \cdot \nabla (\log \rho - c) dx + \int_{\Omega} \rho \nabla c \cdot \nabla (\log \rho - c) dx \\ &= - \int_{\Omega} \rho |\nabla (\log \rho - c)|^2 dx \leq 0, \end{aligned}$$

and therefore we have the desired decrease of the energy in time. $\square$

Our goal is now to formulate a fully discrete numerical scheme based on spatial finite element discretization and implicit Euler time-stepping, which can reproduce all of these properties at the temporally semidiscrete-level upon passing to the limit with the spatial discretization parameter. We shall then pass to the limit with the time-step, while keeping the essential estimates intact in the limit, to establish the existence of a weak solution to the initial-boundary-value problem (1.4), and rigorously prove the decrease in time of the energy.

In order to build our numerical scheme for equation (1.4) that mimics the properties exhibited by ρ , because the assumption that $\rho \geq 0$ played an important role in the derivation of the previous energy estimate, we introduce for $0 < \delta < 1 < L < \infty$ the positive cut-off function $\beta_{\delta}^L \in C^{0,1}(\mathbb{R})$ in the weak formulation (1.7a) via

$$\beta_{\delta}^L(r) := \begin{cases} \delta & \text{if } r \leq \delta, \\ r & \text{if } \delta < r < L, \\ L & \text{if } r \geq L, \end{cases} \quad (1.12)$$

prior to discretizing the problem. The two cut-off parameters, δ and L , will be present in the statement and the analysis of the fully discrete approximation of our model in Section 1.2. We will then take the limit as the lower cut-off parameter δ and the spatial discretization parameter tend to zero, and in Section 1.3 we will make the semidiscrete-in-time approximation independent of the upper cut-off parameter L by establishing a bound on the $L^{\infty}(\Omega)$ norm, which is uniform with respect to L and analogous to the one in Lemma 1.2. In view of this, we also introduce the function $\beta^L \in C(\mathbb{R}_{\geq 0})$, defined as $\beta^L(r) := \min\{r, L\}$ for $r \in \mathbb{R}_{\geq 0}$.

We therefore introduce the following ‘truncated’ weak formulation:

$$\begin{aligned} &\text{Find } \rho_{\delta,L} \in L^2(0, T; V) \text{ with } \frac{\partial \rho_{\delta,L}}{\partial t} \in L^2(0, T; V') \text{ such that} \\ &\left\langle \frac{\partial \rho_{\delta,L}}{\partial t}, \phi \right\rangle = - \int_{\Omega} \nabla \rho_{\delta,L} \cdot \nabla \phi \, dx + \int_{\Omega} \beta_{\delta}^L(\rho_{\delta,L}) \nabla c_{\delta,L} \cdot \nabla \phi \, dx \\ &\quad \text{for all } \phi \in V \text{ and a.e. } t \in (0, T], \end{aligned} \quad (1.13a)$$

subject to the initial condition $\rho_{\delta,L}(\cdot, 0) = \rho_0$, where

$$-(-\Delta_N)^s c_{\delta,L} = \rho_{\delta,L}^* \quad \text{in } \Omega, \quad (1.13b)$$

and, as before, $V = H^1(\Omega)$. In this case, similarly as before, we assume that a solution $\rho_{\delta,L}$ to our regularised problem exists and that it has all the regularity properties that we need for the formal computations that follow.

The structure of the problem (1.13a) is such that it still preserves decay of the energy in time. To confirm this, we introduce a regularised version $G_{\delta}^L \in C^{2,1}(\mathbb{R})$ of the function $G(\cdot)$, defined, for $0 < \delta < 1 < L < \infty$, by

$$G_{\delta}^L(r) := \begin{cases} \frac{r^2 - \delta^2}{2\delta} + (\log \delta - 1)r + 1 & \text{if } r \leq \delta, \\ G(r) & \text{if } \delta < r < L, \\ \frac{r^2 - L^2}{2L} + (\log L - 1)r + 1 & \text{if } r \geq L. \end{cases}$$

Clearly,

$$(G_{\delta}^L)'(r) = \begin{cases} \frac{r}{\delta} + \log \delta - 1 & \text{if } r \leq \delta, \\ \log r & \text{if } \delta < r < L, \\ \frac{r}{L} + \log L - 1 & \text{if } r \geq L, \end{cases} \quad (G_{\delta}^L)''(r) = \begin{cases} \frac{1}{\delta} & \text{if } r \leq \delta, \\ \frac{1}{r} & \text{if } \delta < r < L, \\ \frac{1}{L} & \text{if } r \geq L, \end{cases}$$

and therefore

$$\beta_{\delta}^L(r)(G_{\delta}^L)''(r) = 1 \quad \text{for all } r \in \mathbb{R}.$$

In addition, for any sufficiently smooth function ϕ , the following equality holds (see [23]):

$$\beta_{\delta}^L(\phi) \nabla[(G_{\delta}^L)'(\phi)] = \nabla \phi. \quad (1.14)$$

Moreover, we have that

$$\min\{G_{\delta}^L(r), r(G_{\delta}^L)'(r)\} \geq \begin{cases} \frac{r^2}{2\delta} & \text{if } r \leq 0, \\ \frac{r^2}{4L} - C(L) & \text{if } r \geq 0, \end{cases} \quad (1.15)$$

where $C(L)$ is a positive constant depending only on L . Finally we note that $(G_{\delta}^L)''(r) \geq \frac{1}{L}$ for all $r \in \mathbb{R}$. The regularised version of the energy $E(\rho)$ is then defined by

$$E_{\delta}^L(\rho_{\delta,L}) := \int_{\Omega} G_{\delta}^L(\rho_{\delta,L}) \, dx - \frac{1}{2} \int_{\Omega} \rho_{\delta,L}^* c_{\delta,L} \, dx,$$

and with similar computations as the ones in Lemma 1.3 it is possible to show that

$$\frac{d}{dt} E_{\delta}^L(\rho_{\delta,L}) \leq 0.$$

Remark 1.4. The relationship between the potential and the density expressed by the fractional Poisson equation $-(\Delta_N)^s c_{\delta,L} = \rho_{\delta,L}^*$ will be crucial throughout and we want to highlight now one direct consequence of it, which is the nonpositivity of the L^2 inner product in space between the gradients of $\rho_{\delta,L}$ and $c_{\delta,L}$, namely

$$\int_{\Omega} \nabla \rho_{\delta,L} \cdot \nabla c_{\delta,L} \, dx \leq 0. \quad (1.16)$$

Indeed, by using the definition of the Neumann Laplacian $-\Delta_N$ and recalling that $c_{\delta,L} = -(-\Delta_N)^{-s} \rho_{\delta,L}^*$, we get

$$\begin{aligned} \int_{\Omega} \nabla \rho_{\delta,L} \cdot \nabla c_{\delta,L} \, dx &= \int_{\Omega} \nabla \rho_{\delta,L}^* \cdot \nabla c_{\delta,L} \, dx = \int_{\Omega} \rho_{\delta,L}^* (-\Delta_N) c_{\delta,L} \, dx \\ &= - \int_{\Omega} \rho_{\delta,L}^* (-\Delta_N)^{1-s} \rho_{\delta,L}^* \, dx \leq 0. \end{aligned}$$

We can also derive a formal energy bound. Using the weak formulation (1.13a) with $\phi = (G_{\delta}^L)'(\rho_{\delta,L})$ and property (1.14), we have that

$$\begin{aligned} \frac{d}{dt} E_{\delta}^L(\rho_{\delta,L}) &= - \int_{\Omega} (G_{\delta}^L)''(\rho_{\delta,L}) \nabla \rho_{\delta,L} \cdot \nabla \rho_{\delta,L} \, dx \\ &\quad + 2 \int_{\Omega} \nabla \rho_{\delta,L} \cdot \nabla c_{\delta,L} \, dx - \int_{\Omega} \beta_{\delta}^L(\rho_{\delta,L}) \nabla c_{\delta,L} \cdot \nabla c_{\delta,L} \, dx. \end{aligned}$$

By integrating this equality in time from 0 to t for some $t \in (0, T]$, where $T > 0$, and using (1.15) with the assumption that the initial datum is $(\rho_{\delta,L})_0 = \rho_0 \geq 0$, we have that

$$\begin{aligned} \frac{1}{2\delta} \int_{\Omega} [\rho_{\delta,L}]_-^2 \, dx - \frac{1}{2} \int_{\Omega} \rho_{\delta,L}^* c_{\delta,L} \, dx &\leq C(L) - \int_0^t \int_{\Omega} (G_{\delta}^L)''(\rho_{\delta,L}) |\nabla \rho_{\delta,L}|^2 \, dx \\ &\quad + 2 \int_0^t \int_{\Omega} \nabla \rho_{\delta,L} \cdot \nabla c_{\delta,L} \, dx - \int_0^t \int_{\Omega} \beta_{\delta}^L(\rho_{\delta,L}) |\nabla c_{\delta,L}|^2 \, dx. \end{aligned}$$

The property (1.16) then implies that

$$\frac{1}{2\delta} \int_{\Omega} [\rho_{\delta,L}]_-^2 \, dx + \frac{1}{L} \int_0^t \int_{\Omega} |\nabla \rho_{\delta,L}|^2 \, dx - \frac{1}{2} \int_{\Omega} \rho_{\delta,L}^* c_{\delta,L} \, dx + \int_0^t \int_{\Omega} \beta_{\delta}^L(\rho_{\delta,L}) |\nabla c_{\delta,L}|^2 \, dx \leq C(L),$$

which means, taking the supremum over $t \in (0, T)$ and recalling the equality $-(\Delta_N)^s c_{\delta,L} = \rho_{\delta,L}^*$, that we have

$$\begin{aligned} \frac{1}{\delta} \sup_{t \in (0, T)} \int_{\Omega} [\rho_{\delta,L}]_-^2 \, dx + \int_0^T \int_{\Omega} |\nabla \rho_{\delta,L}|^2 \, dx \\ + \sup_{t \in (0, T)} \int_{\Omega} (-\Delta_N)^s c_{\delta,L} c_{\delta,L} \, dx + \int_0^T \int_{\Omega} \beta_{\delta}^L(\rho_{\delta,L}) |\nabla c_{\delta,L}|^2 \, dx \leq C(L). \end{aligned} \quad (1.17)$$

Hence, we arrive at the following bound, which is uniform with respect to the parameter δ :

$$\begin{aligned} \frac{1}{\delta} \sup_{t \in (0, T)} \|[\rho_{\delta,L}]_-\|_{L^2(\Omega)}^2 + \int_0^T \int_{\Omega} |\nabla \rho_{\delta,L}|^2 \, dx \\ + \sup_{t \in (0, T)} \|c_{\delta,L}\|_{\mathbb{H}^s(\Omega)}^2 + \int_0^T \int_{\Omega} \beta_{\delta}^L(\rho_{\delta,L}) |\nabla c_{\delta,L}|^2 \, dx \leq C(L). \end{aligned}$$

A discrete counterpart of this inequality will be used later on to prove nonnegativity of the numerical solution by passing to the limit $\delta \rightarrow 0_+$.

We can also consider the weak formulation (1.13a) with $\phi = \rho_{\delta,L}$. We then have that

$$\int_{\Omega} (\rho_{\delta,L})_t \rho_{\delta,L} \, dx = - \int_{\Omega} |\nabla \rho_{\delta,L}|^2 \, dx + \int_{\Omega} \beta_{\delta}^L(\rho_{\delta,L}) \nabla c_{\delta,L} \cdot \nabla \rho_{\delta,L} \, dx,$$

and the application of the Cauchy–Schwarz inequality and Young’s inequality yields, for any $\eta > 0$, that

$$\frac{1}{2} \frac{d}{dt} \int_{\Omega} \rho_{\delta,L}^2 \, dx \leq - \int_{\Omega} |\nabla \rho_{\delta,L}|^2 \, dx + \frac{\eta}{2} \int_{\Omega} \beta_{\delta}^L(\rho_{\delta,L}) |\nabla \rho_{\delta,L}|^2 \, dx + \frac{1}{2\eta} \int_{\Omega} \beta_{\delta}^L(\rho_{\delta,L}) |\nabla c_{\delta,L}|^2 \, dx.$$

Hence, by taking η sufficiently small and recalling (1.17), we get the following overall bound on $\rho_{\delta,L}$:

$$\sup_{t \in (0,T)} \int_{\Omega} \rho_{\delta,L}^2 \, dx + \frac{1}{\delta} \sup_{t \in (0,T)} \int_{\Omega} [\rho_{\delta,L}]_-^2 \, dx + \int_0^T \int_{\Omega} |\nabla \rho_{\delta,L}|^2 \, dx \leq C(L). \quad (1.18)$$

Motivated by these formal calculations, we shall design a finite element method whose solution mimics the energy law of (1.13) and the formal bounds (1.17) and (1.18) at a discrete level, and show that, as the spatial and temporal discretization parameters tend to zero, a subsequence of this sequence of approximations converges to a bounded and nonnegative weak solution of our original problem in a suitable sense. In doing so, we shall confine ourselves to the physically relevant cases of $d = 2$ and $d = 3$ space dimensions. The arguments that follow can be therefore viewed as a constructive proof of the existence of a nonnegative, energy-dissipative, weak solution to the initial-boundary-value problem for the fractional porous medium equation under consideration, based on the Neumann Laplacian.

1.2 Finite element approximation

We now define the fully discrete scheme for the numerical approximation of the problem (1.13). Our approach is to couple the strategy used in [21, 22, 23] in terms of the spatial finite element scheme with recent results concerning numerical approximation of the fractional Laplacian [38, 39, 43, 44]. The overall aim is to construct a finite element approximation of the problem (1.4) in its weak formulation (1.13), which mimics the estimate (1.17) at a discrete level, and to show that a subsequence of this sequence of approximations converges to a bounded and nonnegative weak solution, first as the spatial discretization parameter h and the lower cut-off parameter δ tend to zero, and then as the time-step Δt tends to zero. It will also transpire that it suffices to take a fixed value of the upper cut-off parameter L such that $L > \|\rho_0\|_{L^\infty(\Omega)}$; passage to the limit $L \rightarrow +\infty$ will therefore not be required. We begin by introducing the spatial finite element approximation.

For ease of triangulating Ω , we shall assume that Ω is a bounded open and convex Lipschitz polygonal domain in $\mathbb{R}^2$ or a bounded open and convex Lipschitz polyhedral domain in $\mathbb{R}^3$.

With $h > 0$ being our spatial discretization parameter, let $\mathcal{T}_h = \{K_n\}_{n=1}^{M_h}$ be a quasi-uniform and shape-regular family of triangulations of $\bar{\Omega}$, where K_n , $n = 1, \dots, M_h$, are closed simplices with mutually disjoint interiors, such that $\bar{\Omega} = \cup_{n=1}^{M_h} K_n$; assume further that the triangulation is weakly acute. We remark that the use of a weakly acute triangulation is essential for our argument, since it underpins the technical results that ensure the nonnegativity of the entropy in the discrete energy inequality. Let V_h be the linear space of continuous piecewise affine functions defined on this triangulation, i.e.,

$$V_h := \{v_h \in C(\bar{\Omega}) \text{ such that } v_h|_K \in \mathbb{P}^1 \text{ for all } K \in \mathcal{T}_h\},$$

and let $N_h := \dim(V_h)$. Moreover, let $\pi_h : C^0(\bar{\Omega}) \rightarrow V_h$ be the interpolation operator into the linear space V_h based on nodal evaluation, i.e., such that, for each $\phi \in C(\bar{\Omega})$,

$$\pi_h \phi(P_j) = \phi(P_j), \quad j = 1, \dots, N_h,$$

where $\{P_j\}_{j=1}^{N_h}$ are the nodes (vertices) of $\mathcal{T}_h$ contained in $\bar{\Omega}$.

In order to construct a discrete version of the fractional spectral Neumann Laplacian we first consider a finite-dimensional approximation, $-\Delta_h$, of the standard Neumann Laplacian $-\Delta_N$. Let us consider the bilinear form

$$a : H_*^1(\Omega) \times H_*^1(\Omega) \rightarrow \mathbb{R} \quad \text{where} \quad a(u, v) := \int_{\Omega} \nabla u \cdot \nabla v \, dx, \quad (1.19)$$

which is symmetric, bounded and coercive; we can restrict $a(\cdot, \cdot)$ to $(V_h \cap L_*^2(\Omega)) \times (V_h \cap L_*^2(\Omega))$. Clearly, $V_h \cap L_*^2(\Omega) (= V_h \cap H_*^1(\Omega))$ is an $(N_h - 1)$ -dimensional linear subspace of $H_*^1(\Omega)$. The bilinear form (1.19) gives rise in $V_h \cap L_*^2(\Omega)$ to a discrete orthonormal basis of eigenfunctions that we denote by $\{\varphi_k^h\}_{k=1}^{N_h-1}$ with corresponding positive eigenvalues $\lambda_1^h, \dots, \lambda_{N_h-1}^h$ such that

$$a(\varphi_k^h, v_h) = \lambda_k^h(\varphi_k^h, v_h) \quad \text{for all } v_h \in V_h \cap L_*^2(\Omega), \quad k = 1, \dots, N_h - 1.$$

Using these eigenpairs, we can now propose a similar expression to (1.5) and introduce a finite-dimensional counterpart of the fractional spectral Neumann Laplacian, $(-\Delta_N)^s$; namely, for $u_h \in V_h \cap L_*^2(\Omega)$ and $s \in [0, 1]$, we define

$$(-\Delta_h)^s u_h := \sum_{k=1}^{N_h-1} (\lambda_k^h)^s u_k^h \varphi_k^h \quad \text{with } u_k^h := \int_{\Omega} u_h \varphi_k^h \, dx, \quad k = 1, \dots, N_h - 1. \quad (1.20)$$

Remark 1.5. We notice that this definition is consistent with the definition of $-\Delta_h$, in the sense that if $s = 1$ then

$$(-\Delta_h) u_h = \sum_{k=1}^{N_h-1} \lambda_k^h u_k^h \varphi_k^h \quad \text{with } u_k^h = \int_{\Omega} u_h \varphi_k^h \, dx, \quad k = 1, \dots, N_h - 1,$$

and

$$((-\Delta_h) u_h, v_h) = \sum_{k=1}^{N_h-1} u_k^h \lambda_k^h (\varphi_k^h, v_h) = \sum_{k=1}^{N_h-1} u_k^h a(\varphi_k^h, v_h) = a(u_h, v_h).$$

We shall also define the finite element approximation, T_h , of the inverse spectral Neumann Laplacian $T = (-\Delta_N)^{-1}$, that for each $F \in H^{-1}(\Omega)$ (uniquely) associates $T_h(F) := u_h \in V_h \cap L_*^2(\Omega)$ such that

$$a(u_h, v_h) = \langle F, v_h \rangle, \quad \text{for all } v_h \in V_h \cap L_*^2(\Omega).$$

We shall require in the analysis of our fully discrete numerical method a discrete version of the property (1.14). In order to ensure that this holds, we define a diagonal matrix $\Theta_\delta^L(\phi_h) \in \mathbb{R}^{d \times d}$ in the following way: for an element $K \in \mathcal{T}_h$, let $\{P_i\}_{i=0}^d$ be the vertices of the simplex K ; then, for $j = 1, \dots, d$ and $x \in K^\circ$ (the interior of K), we define

$$\tilde{\Theta}_\delta^L(\phi_h)_{jj}(x) := \begin{cases} \frac{\phi_h(P_j) - \phi_h(P_0)}{(G_\delta^L)'(\phi_h(P_j)) - (G_\delta^L)'(\phi_h(P_0))} & \text{if } \phi_h(P_j) \neq \phi_h(P_0), \\ \frac{1}{(G_\delta^L)''(\phi_h(P_j))} = \beta_\delta^L(\phi_h(P_j)) & \text{if } \phi_h(P_j) = \phi_h(P_0). \end{cases} \quad (1.21a)$$

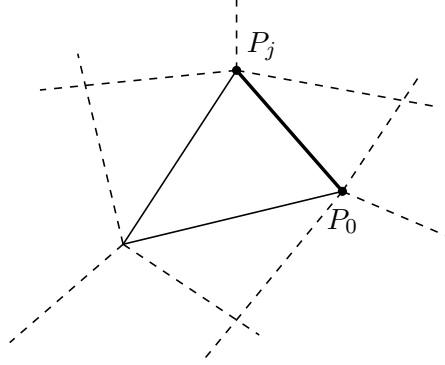


Figure 1.1: Triangulation and the computation of the matrix $\tilde{\Theta}_\delta^L$

The matrix $\tilde{\Theta}_\delta^L$ is designed to approximate $\beta_\delta^L I$, where β_δ^L is the positive cut-off function defined above, and its elements are simply difference quotients approximating the inverse of the derivative of $(G_\delta^L)'$, which is $(\beta_\delta^L)^{-1}$.

Now, let $\hat{K}$ be the reference simplex and $\hat{x} \in \hat{K} \mapsto P_0 + B_K \hat{x} = x \in K$ the affine function that maps $\hat{K}$ onto K , and for $x \in K^\circ$ define

$$\Theta_\delta^L(\phi_h)(x) := (B_K^T)^{-1} \tilde{\Theta}_\delta^L(\phi_h)(x) B_K^T. \quad (1.21b)$$

With this definition in place we have that

$$\Theta_\delta^L(\phi_h)(x) \nabla[\pi_h((G_\delta^L)'(\phi_h))(x)] = \nabla \phi_h(x) \quad \text{for all } x \in K^\circ. \quad (1.22)$$

The construction of such a matrix, used in [23], goes back to [115, 20].

The proof of the following lemma is a simple extension of the proof of [20, Lemma 2.1] and is therefore omitted.

Lemma 1.6. Let $\|\cdot\|$ denote the spectral norm on $\mathbb{R}^{d \times d}$. For any $\delta \in (0, 1)$ and $L > 1$ the function $\Theta_\delta^L : V_h \rightarrow \mathbb{R}^{d \times d}$ is continuous, and for every $K \in \mathcal{T}_h$ and every $x \in K^\circ$ it holds

$$|\xi^T \Theta_\delta^L(\phi_h)(x) \xi| \leq \kappa_2(B_K) L \xi^T \xi \quad \text{for all } \xi \in \mathbb{R}^d, \phi_h \in V_h,$$

where $\kappa_2(B_K) = \|B_K\| \|B_K^{-1}\|$. Furthermore, for all $\phi_h^{(1)}, \phi_h^{(2)} \in V_h$ and all $K \in \mathcal{T}_h$, one has that

$$\|(\Theta_\delta^L(\phi_h^{(1)}) - \Theta_\delta^L(\phi_h^{(2)}))(x)\| \leq \kappa_2(B_K) \frac{L}{\delta} \max_{j=1, \dots, d} (|\phi_h^{(1)}(P_j) - \phi_h^{(2)}(P_j)| + |\phi_h^{(1)}(P_0) - \phi_h^{(2)}(P_0)|)$$

for all $x \in K^\circ$.

Moreover, it is possible to prove the following lemma (the proof can be found in [22]), which clarifies the sense in which the matrix function $\Theta_\delta^L(\cdot)$ approximates the cut-off function $\beta_\delta^L(\cdot)I$, as δ and h tend to zero.

Lemma 1.7. For each $K \in \mathcal{T}_h$ and for all $\phi_h \in V_h$ we have that

$$\int_K |\Theta_\delta^L(\phi_h) - \beta_\delta^L(\phi_h)I|^2 dx \leq C \left(\delta^2 + h^2 \int_K |\nabla \phi_h|^2 dx + \int_K \pi_h([\phi_h]_-^2) dx \right).$$

The following lemma, together with its corollary, were also proved in [22]; they will be crucial in our argument to show convergence of a subsequence as h and δ tend to zero and we therefore report them here.

Lemma 1.8. Let $g \in C^{0,1}(\mathbb{R})$ be monotonically increasing with Lipschitz constant g_{Lip} ; then, for all $K \in \mathcal{T}_h$ and for all $\phi_h \in V_h$,

$$\int_K |\nabla(\pi_h(g(\phi_h)))|^2 dx \leq g_{\text{Lip}} \int_K \nabla \phi_h \cdot \nabla \pi_h(g(\phi_h)) dx.$$

Corollary 1.9. Let g be a function defined and strictly monotonically increasing on $\mathbb{R}$, such that g^{-1} , the inverse function of g , is Lipschitz continuous on $\mathbb{R}$, with Lipschitz constant $(g^{-1})_{\text{Lip}}$; then, for all $K \in \mathcal{T}_h$ and for all $\phi_h \in V_h$,

$$\int_K |\nabla \phi_h|^2 dx \leq (g^{-1})_{\text{Lip}} \int_K \nabla \phi_h \cdot \nabla \pi_h(g(\phi_h)) dx.$$

We further note that, for each $K \in \mathcal{T}_h$ with vertices $\{P_j\}_{j=0}^d$, by virtue of Jensen's inequality we have

$$(\pi_h(\phi)(x))^2 = \left(\sum_{j=0}^d \phi(P_j) \phi_j(x) \right)^2 \leq \sum_{j=0}^d (\phi(P_j))^2 \phi_j(x) = \pi_h(\phi^2)(x) \quad (1.23)$$

for all $x \in K$ and all $\phi \in C(\overline{K})$.

In order to formulate the discretization of the problem under consideration with respect to the temporal variable, we let $T > 0$ denote the final time and we introduce a temporal mesh given by $0 =: t_0 < t_1 < \dots < t_N := T$, which for the ease of exposition we choose to be uniform, with spacing Δt ; i.e., $t_n - t_{n-1} = \Delta t$ for all $n = 1, \dots, N$.

Given the initial datum $\rho_0 \in L^\infty(\Omega)$ such that $\rho_0 \geq 0$ and $\frac{1}{|\Omega|} \int_\Omega \rho_0 \, dx = 1$, we first choose $\rho_h^0 \in V_h$ as the unique solution of the following problem:

$$\int_\Omega \pi_h(\rho_h^0 \phi_h) \, dx + \Delta t \int_\Omega \nabla \rho_h^0 \cdot \nabla \phi_h \, dx = \int_\Omega \rho_0 \phi_h \, dx \quad \text{for all } \phi_h \in V_h, \quad (1.24)$$

in order to have an $H^1(\Omega)$ regularisation of the initial datum. The existence of a unique solution $\rho_h^0 \in V_h$ to (1.24) is a consequence of the fact that (1.24) is equivalent to a system of linear algebraic equations with a symmetric positive definite matrix. By taking $\phi_h = \rho_h^0$ in (1.24), it follows using (1.23) and Young's inequality that

$$\int_\Omega (\rho_h^0)^2 \, dx + 2\Delta t \int_\Omega |\nabla \rho_h^0|^2 \, dx \leq \int_\Omega \rho_0^2 \, dx \leq |\Omega| \|\rho_0\|_{L^\infty(\Omega)}^2. \quad (1.25)$$

Furthermore, by taking $\phi_h \equiv 1 \in V_h$ in (1.24) and noting that $\pi_h \rho_h^0 = \rho_h^0$, it follows that

$$\frac{1}{|\Omega|} \int_\Omega \rho_h^0(x) \, dx = \frac{1}{|\Omega|} \int_\Omega \rho_0(x) \, dx = 1.$$

Next, we shall prove that $0 \leq \rho_h^0(x) \leq \|\rho_0\|_{L^\infty(\Omega)}$ for all $x \in \bar{\Omega}$. To this end, we consider the function φ_p , defined so that its first derivative is a regularised version of the function $r \in \mathbb{R} \mapsto [r]_- \in \mathbb{R}_{\leq 0}$. More precisely, for $p > 0$, we consider

$$\varphi_p(r) := \begin{cases} \frac{r^2}{2} + \frac{r}{2p} + \frac{1}{6p^2} & \text{if } r \leq -\frac{1}{p}, \\ -\frac{pr^3}{6} & \text{if } -\frac{1}{p} \leq r \leq 0, \\ 0 & \text{if } r \geq 0. \end{cases}$$

The first and second derivative of φ_p are then given by, respectively,

$$\varphi_p'(r) = \begin{cases} r + \frac{1}{2p} & \text{if } r \leq -\frac{1}{p}, \\ -\frac{pr^2}{2} & \text{if } -\frac{1}{p} \leq r \leq 0, \\ 0 & \text{if } r \geq 0; \end{cases} \quad \varphi_p''(r) = \begin{cases} 1 & \text{if } r \leq -\frac{1}{p}, \\ -pr & \text{if } -\frac{1}{p} \leq r \leq 0, \\ 0 & \text{if } r \geq 0. \end{cases}$$

Clearly, $\varphi_p \in C^{2,1}(\mathbb{R})$ and φ_p is a nonnegative convex function. Furthermore, $\varphi_p'(r) \leq 0$ and $r\varphi_p'(r) \geq 0$ for all $r \in \mathbb{R}$.

We then take $\phi_h = \pi_h(\varphi_p'(\rho_h^0))$ as test function in (1.24) and apply Lemma 1.8 to infer that with this choice of ϕ_h the second term on the left-hand side of (1.24) is nonnegative, and therefore

$$\int_\Omega \pi_h(\rho_h^0 \pi_h(\varphi_p'(\rho_h^0))) \, dx \leq \int_\Omega \rho_0 \pi_h(\varphi_p'(\rho_h^0)) \, dx \leq 0,$$

because, by hypothesis, $\rho_0(x) \geq 0$ for a.e. $x \in \Omega$ while $\pi_h(\varphi_p'(\rho_h^0(x))) \leq 0$ for all $x \in \bar{\Omega}$ since $\varphi_p'(\rho_h^0(x)) \leq 0$ for all $x \in \bar{\Omega}$. On the other hand,

$$0 \leq \int_\Omega \pi_h(\rho_h^0 \varphi_p'(\rho_h^0)) \, dx = \int_\Omega \pi_h(\rho_h^0 \pi_h(\varphi_p'(\rho_h^0))) \, dx \leq 0,$$

because $\rho_h^0(x) \varphi_p'(\rho_h^0(x)) \geq 0$ for all $x \in \bar{\Omega}$. Hence,

$$\int_\Omega \pi_h(\rho_h^0 \varphi_p'(\rho_h^0)) \, dx = 0.$$

Passing to the limit $p \rightarrow +\infty$, this implies that

$$\int_{\Omega} \pi_h(\rho_h^0 [\rho_h^0]_-) dx = 0.$$

As $\pi_h(\rho_h^0 [\rho_h^0]_-) = \pi_h(([\rho_h^0]_-)^2)$ and the latter is a nonnegative function on $\bar{\Omega}$, we deduce that $\pi_h(([\rho_h^0]_-)^2)$ is identically zero on $\bar{\Omega}$; equivalently, $([\rho_h^0]_-)^2(P_j) = 0$ at all vertices P_j , $j = 1, \dots, N_h$, of the triangulation. Therefore, $\rho_h^0(P_j) \geq 0$ for all $j = 1, \dots, N_h$, and consequently, because ρ_h^0 is piecewise affine, $\rho_h^0(x) \geq 0$ for all $x \in \bar{\Omega}$.

One can use an analogous argument to show that $\rho_h^0 \leq \|\rho_0\|_{L^\infty(\Omega)}$ on $\bar{\Omega}$. Indeed, if we define $A := \|\rho_0\|_{L^\infty(\Omega)}$ and the functions $\hat{\rho}_h^0 := A - \rho_h^0$ and $\hat{\rho}_0 := A - \rho_0$, then, because $\pi_h \phi_h = \phi_h$ for all $\phi_h \in V_h$, it follows from (1.24) that

$$\int_{\Omega} \pi_h(\hat{\rho}_h^0 \phi_h) dx + \Delta t \int_{\Omega} \nabla \hat{\rho}_h^0 \cdot \nabla \phi_h dx = \int_{\Omega} \hat{\rho}_0 \phi_h dx \quad \text{for all } \phi_h \in V_h.$$

As $\hat{\rho}_0 \geq 0$ a.e. on Ω , an identical argument to the one above implies that $\hat{\rho}_h^0 \geq 0$ on $\bar{\Omega}$, whereby $\rho_h^0 \leq A = \|\rho_0\|_{L^\infty(\Omega)}$, as required. To summarize, we have shown that

$$0 \leq \rho_h^0(x) \leq \|\rho_0\|_{L^\infty(\Omega)} \quad \text{for all } x \in \bar{\Omega} \quad \text{and} \quad \frac{1}{|\Omega|} \int_{\Omega} \rho_h^0(x) dx = 1. \quad (1.26)$$

With ρ_h^0 thus defined, the fully-discrete scheme for the problem under consideration is then the following: ¹

$$\begin{aligned} &\text{Let } \rho_{h,\delta,L}^0 := \rho_h^0 \in V_h. \text{ For } n = 1, \dots, N, \text{ given } \rho_{h,\delta,L}^{n-1} \in V_h, \text{ find } \rho_{h,\delta,L}^n \in V_h \text{ such that} \\ &\int_{\Omega} \pi_h \left(\frac{\rho_{h,\delta,L}^n - \rho_{h,\delta,L}^{n-1}}{\Delta t} \phi_h \right) dx = - \int_{\Omega} \nabla \rho_{h,\delta,L}^n \cdot \nabla \phi_h dx + \int_{\Omega} \nabla c_{h,\delta,L}^n \cdot \Theta_{\delta}^L(\rho_{h,\delta,L}^n) \nabla \phi_h dx \quad (1.27a) \\ &\text{for all } \phi_h \in V_h, \end{aligned}$$

where $c_{h,\delta,L}^n \in V_h \cap L_*^2(\Omega)$ satisfies

$$-(-\Delta_h)^s c_{h,\delta,L}^n = (\rho_{h,\delta,L}^n)^*. \quad (1.27b)$$

The time-stepping scheme is chosen to be implicit and we stress that the numerical approximation relies on the potential $c_{h,\delta,L}$ and the fact that it is repulsive in the sense that (1.16) holds. This will be crucial in deriving global-in-time existence, uniform boundedness and convergence of the sequence of numerical solutions.

Since our first analytical step is to pass to the limit as $\delta, h \rightarrow 0_+$, we now introduce the definition of the semidiscrete-in-time approximation of our problem, to which the fully discrete scheme (1.27) will be shown to converge in this limit. We first need to assign to $\rho_0 \in L^\infty(\Omega)$,

¹Lemma 1.6 and the scheme in the form stated in (1.27) correct a technical slip present in [62]. The correction has no impact on the correctness of the main results of [62].

for a fixed value of $\Delta t > 0$, a certain smoothed initial datum $\rho^0 = \rho^0(\Delta t) \in V = H^1(\Omega)$, that is the solution to the following problem:

$$\int_{\Omega} \rho^0 \phi \, dx + \Delta t \int_{\Omega} \nabla \rho^0 \cdot \nabla \phi \, dx = \int_{\Omega} \rho_0 \phi \, dx \quad \text{for all } \phi \in V. \quad (1.28)$$

It follows by an application of the Lax–Milgram lemma that (1.28) has a unique solution $\rho^0 = \rho^0(\Delta t) \in V = H^1(\Omega)$. By taking $\phi \equiv 1$ we find that $\frac{1}{|\Omega|} \int_{\Omega} \rho^0 \, dx = \frac{1}{|\Omega|} \int_{\Omega} \rho_0 \, dx = 1$. Furthermore, one can show that the following four assertions hold true:

$$\rho^0 \rightarrow \rho_0 \quad \text{weakly in } L^2(\Omega) \quad \text{as } \Delta t \rightarrow 0_+;$$

thanks to the assumed nonnegativity of ρ_0 also $\rho^0 \geq 0$ a.e. on Ω ; the function ρ^0 satisfies

$$\int_{\Omega} G(\rho^0) \, dx + 4\Delta t \int_{\Omega} \left| \nabla \sqrt{\rho^0} \right|^2 \, dx \leq \int_{\Omega} G(\rho_0) \, dx, \quad (1.29)$$

where $G \in C([0, \infty))$ is the nonnegative convex function defined in (1.9); and $\rho^0 \in L^\infty(\Omega) \cap V$. The full details of the proofs of these assertions are contained in the Appendix of [23] and in [21, Section 6].

With this definition of $\rho^0 = \rho^0(\Delta t)$ the semidiscrete-in-time approximation of our problem is then formulated as follows:

$$\begin{aligned} &\text{Let } \rho_L^0 := \rho^0 = \rho^0(\Delta t). \text{ For } n = 1, \dots, N, \text{ given } \rho_L^{n-1} \in V, \text{ find } \rho_L^n \in V \text{ such that} \\ &\int_{\Omega} \frac{\rho_L^n - \rho_L^{n-1}}{\Delta t} \phi \, dx = - \int_{\Omega} \nabla \rho_L^n \cdot \nabla \phi \, dx + \int_{\Omega} \beta^L(\rho_L^n) \nabla c_L^n \cdot \nabla \phi \, dx \quad \text{for all } \phi \in V, \end{aligned} \quad (1.30a)$$

subject to the initial condition $\rho_L^0 = \rho^0$, where

$$-(-\Delta_N)^s c_L^n = (\rho_L^n)^* \quad \text{in } \Omega. \quad (1.30b)$$

1.2.1 Convergence analysis of the discretized fractional porous medium model

Our aim in the rest of this section is to pass to the limit in (1.27a), (1.27b) as δ and h tend to zero, to infer the semidiscrete-in-time approximation (1.30a), (1.30b) as the limiting problem. The analysis of the semidiscrete-in-time approximation will then be the focus of the next section, where we shall pass to the limit $\Delta t \rightarrow 0_+$ in (1.30a), (1.30b), and will also show that the sequence of approximations becomes independent of L once $L > \|\rho_0\|_{L^\infty(\Omega)}$, which then makes passage to the limit $L \rightarrow +\infty$ redundant. The first result we prove is an a priori bound on the solution $\rho_{h,\delta,L}^n$ of (1.27a), assuming that it exists, with the existence of a solution to be proved thereafter.

Lemma 1.10. *For $n = 1, \dots, N$ a solution $\rho_{h,\delta,L}^n \in V_h$ of (1.27a), if it exists, satisfies the following bound:*

$$\int_{\Omega} \pi_h(G_\delta^L(\rho_{h,\delta,L}^n)) \, dx + \Delta t \int_{\Omega} \nabla \rho_{h,\delta,L}^n \cdot \nabla \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) \, dx \leq \int_{\Omega} \pi_h(G_\delta^L(\rho_{h,\delta,L}^{n-1})) \, dx. \quad (1.31)$$

Proof. By taking $\phi_h = \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n))$ as test function in (1.27a), we have that

$$\begin{aligned} \int_{\Omega} \pi_h \left(\frac{\rho_{h,\delta,L}^n - \rho_{h,\delta,L}^{n-1}}{\Delta t} \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) \right) dx &= - \int_{\Omega} \nabla \rho_{h,\delta,L}^n \cdot \nabla \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) dx \\ &\quad + \int_{\Omega} \nabla c_{h,\delta,L}^n \cdot \Theta_\delta^L(\rho_{h,\delta,L}^n) \nabla \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) dx. \end{aligned}$$

Hence, by (1.22), it follows that

$$\begin{aligned} \int_{\Omega} \pi_h \left(\frac{\rho_{h,\delta,L}^n - \rho_{h,\delta,L}^{n-1}}{\Delta t} \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) \right) dx &= - \int_{\Omega} \nabla \rho_{h,\delta,L}^n \cdot \nabla \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) dx \\ &\quad + \int_{\Omega} \nabla c_{h,\delta,L}^n \cdot \nabla \rho_{h,\delta,L}^n dx. \end{aligned}$$

Next, we bound the left-hand side of this equality from below by using the convexity of G_δ^L , which implies that

$$\begin{aligned} \pi_h \left((\rho_{h,\delta,L}^n - \rho_{h,\delta,L}^{n-1}) \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) \right) &= \pi_h \left((\rho_{h,\delta,L}^n - \rho_{h,\delta,L}^{n-1}) (G_\delta^L)'(\rho_{h,\delta,L}^n) \right) \\ &\geq \pi_h \left(G_\delta^L(\rho_{h,\delta,L}^n) - G_\delta^L(\rho_{h,\delta,L}^{n-1}) \right) \\ &= \pi_h(G_\delta^L(\rho_{h,\delta,L}^n)) - \pi_h(G_\delta^L(\rho_{h,\delta,L}^{n-1})), \end{aligned}$$

and therefore

$$\begin{aligned} \frac{1}{\Delta t} \int_{\Omega} (\pi_h(G_\delta^L(\rho_{h,\delta,L}^n)) - \pi_h(G_\delta^L(\rho_{h,\delta,L}^{n-1}))) dx &+ \int_{\Omega} \nabla \rho_{h,\delta,L}^n \cdot \nabla \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) dx \\ &\leq \int_{\Omega} \nabla c_{h,\delta,L}^n \cdot \nabla \rho_{h,\delta,L}^n dx. \end{aligned} \quad (1.32)$$

We observe that, in the case of a repulsive potential under consideration here, the right-hand side of inequality (1.32) contributes ‘constructively’ to the desired bound, in the sense that it satisfies

$$\int_{\Omega} \nabla c_{h,\delta,L}^n \cdot \nabla \rho_{h,\delta,L}^n dx \leq 0. \quad (1.33)$$

Indeed, thanks to the definition of the finite element approximation of the fractional Laplacian stated in equation (1.20), we have that

$$\begin{aligned} \int_{\Omega} \nabla c_{h,\delta,L}^n \cdot \nabla \rho_{h,\delta,L}^n dx &= \int_{\Omega} \nabla c_{h,\delta,L}^n \cdot \nabla (\rho_{h,\delta,L}^n)^* dx = a(c_{h,\delta,L}^n, (\rho_{h,\delta,L}^n)^*) \\ &= a(c_{h,\delta,L}^n, -(-\Delta_h)^s c_{h,\delta,L}^n) = - \sum_{k=1}^{N_h-1} (\lambda_k^h)^s (c_{h,\delta,L}^n)_k a(c_{h,\delta,L}^n, \phi_k^h) \\ &= - \sum_{k=1}^{N_h-1} (\lambda_k^h)^{1+s} (c_{h,\delta,L}^n)_k^2 \leq 0. \end{aligned}$$

This then completes the proof of the lemma. $\square$

We shall now prove the existence of a solution at a given time t_n in order to be able to use the bound (1.31). We will do so by using Brouwer's fixed point theorem.

Lemma 1.11. *For any $\Delta t > 0$, given $\rho_{h,\delta,L}^{n-1} \in V_h$, there exists at least one solution $(\rho_{h,\delta,L}^n, c_{h,\delta,L}^n) \in V_h \times (V_h \cap L_*^2(\Omega))$ to (1.27).*

Proof. We begin by equipping V_h with the inner product $((\cdot, \cdot))$, defined by

$$((\psi_h, \phi_h)) := \int_{\Omega} \pi_h(\psi_h(x)\phi_h(x)) \, dx, \quad \psi_h, \phi_h \in V_h.$$

Next, we define the function $\mathcal{H} : V_h \rightarrow V_h$ such that, for any $\rho_h \in V_h$,

$$((\mathcal{H}(\rho_h), \phi_h)) := \int_{\Omega} \pi_h \left(\frac{\rho_h - \rho_{h,\delta,L}^{n-1}}{\Delta t} \phi_h \right) \, dx + \int_{\Omega} \nabla \rho_h \cdot \nabla \phi_h \, dx - \int_{\Omega} \nabla c_h \cdot \Theta_{\delta}^L(\rho_h) \nabla \phi_h \, dx$$

for all $\phi_h \in V_h$, where $c_h \in V_h \cap L_*^2(\Omega)$ satisfies $-(-\Delta_h)^s c_h = \rho_h^*$. The construction of Θ_{δ}^L , together with Lemma 1.6, ensures that $\mathcal{H}$ is a continuous mapping. Note that if a solution $\rho_{h,\delta,L}^n$ to (1.27a) exists then it is a zero of $\mathcal{H}$, namely

$$((\mathcal{H}(\rho_{h,\delta,L}^n), \phi_h)) = 0 \quad \text{for all } \phi_h \in V_h.$$

We shall therefore prove that $\mathcal{H}$ has a zero. For contradiction, let us assume that $\mathcal{H}$ has no zero for any $\gamma \in \mathbb{R}_{>0}$ in the ball $B_{\gamma} = \{\psi_h \in V_h \text{ such that } \|\psi_h\|_{L^2(\Omega)} \leq \gamma\}$. We define the function $\mathcal{E}_{\gamma} : B_{\gamma} \rightarrow B_{\gamma}$ by

$$\mathcal{E}_{\gamma}(\psi_h) = -\gamma \frac{\mathcal{H}(\psi_h)}{\|\mathcal{H}(\psi_h)\|_{L^2(\Omega)}}.$$

By Brouwer's fixed point theorem $\mathcal{E}_{\gamma}$ has at least one fixed point ρ_h^{γ} in B_{γ} , and this means that $\|\rho_h^{\gamma}\|_{L^2(\Omega)} = \|\mathcal{E}_{\gamma}(\rho_h^{\gamma})\|_{L^2(\Omega)} = \gamma$. Let c_h^{γ} be the solution of the equation $-(-\Delta_h)^s c_h^{\gamma} = (\rho_h^{\gamma})^*$ in Ω . Now let us choose $\phi_h = \pi_h((G_{\delta}^L)'(\rho_h^{\gamma}))$ as test function and notice that, by (1.15) and inequality (1.23), together with the trivial equality $\pi_h \rho_h^{\gamma} = \rho_h^{\gamma}$, we have that

$$\begin{aligned} ((\mathcal{H}(\rho_h^{\gamma}), \pi_h((G_{\delta}^L)'(\rho_h^{\gamma})))) &= -\frac{\|\mathcal{H}(\rho_h^{\gamma})\|_{L^2(\Omega)}}{\gamma} \left(\int_{\Omega} \pi_h(\rho_h^{\gamma}) \pi_h((G_{\delta}^L)'(\rho_h^{\gamma})) \, dx \right) \\ &= -\frac{\|\mathcal{H}(\rho_h^{\gamma})\|_{L^2(\Omega)}}{\gamma} \left(\int_{\Omega} \pi_h(\rho_h^{\gamma}) (G_{\delta}^L)'(\rho_h^{\gamma}) \, dx \right) \\ &\leq -\frac{\|\mathcal{H}(\rho_h^{\gamma})\|_{L^2(\Omega)}}{\gamma} \left(\int_{\Omega} \left(\frac{(\rho_h^{\gamma})^2}{4L} - C(L) \right) \, dx \right) \\ &= -\frac{\|\mathcal{H}(\rho_h^{\gamma})\|_{L^2(\Omega)}}{\gamma} \left(\frac{\gamma^2}{4L} - C(L)|\Omega| \right), \end{aligned}$$

and thus for $\gamma > [4L C(L) |\Omega|]^{1/2}$ we have that

$$((\mathcal{H}(\rho_h^{\gamma}), \pi_h(G_{\delta}^L)'(\rho_h^{\gamma}))) < 0.$$

On the other hand, we can proceed in a similar way as in Lemma 1.10 to deduce that

$$\begin{aligned}
((\mathcal{H}(\rho_h^\gamma), \pi_h(G_\delta^L)'(\rho_h^\gamma))) &= \frac{1}{\Delta t} \int_{\Omega} \pi_h((\rho_h^\gamma - \rho_{h,\delta,L}^{n-1}) \pi_h((G_\delta^L)'(\rho_h^\gamma))) \, dx \\
&\quad + \int_{\Omega} \nabla \rho_h^\gamma \cdot \nabla \pi_h((G_\delta^L)'(\rho_h^\gamma)) \, dx \\
&\quad - \int_{\Omega} \nabla c_h^\gamma \cdot \Theta_\delta^L(\rho_h^\gamma) \nabla \pi_h((G_\delta^L)'(\rho_h^\gamma)) \, dx \\
&\geq \underbrace{\frac{1}{\Delta t} \int_{\Omega} \pi_h((\rho_h^\gamma - \rho_{h,\delta,L}^{n-1}) \pi_h((G_\delta^L)'(\rho_h^\gamma))) \, dx}_{\textcircled{1}} - \underbrace{\int_{\Omega} \nabla c_h^\gamma \cdot \nabla \rho_h^\gamma \, dx}_{\textcircled{2}}. \quad (1.34)
\end{aligned}$$

For the first term in (1.34) we can use the convexity of G_δ^L to deduce, as in the proof of the previous lemma, that

$$\begin{aligned}
\textcircled{1} &\geq \frac{1}{\Delta t} \int_{\Omega} \left(\pi_h(G_\delta^L(\rho_h^\gamma)) - \pi_h(G_\delta^L(\rho_h^{n-1})) \right) \, dx \\
&\geq \frac{1}{\Delta t} \left(\frac{\gamma^2}{4L} - C(L)|\Omega| \right) - \frac{1}{\Delta t} \int_{\Omega} \pi_h(G_\delta^L(\rho_h^{n-1})) \, dx.
\end{aligned}$$

For the second term in (1.34) we can use the definition of c_h^γ involving the discrete fractional Neumann Laplacian to deduce an inequality analogous to (1.33), which then implies that $\textcircled{2} \geq 0$. Therefore,

$$((\mathcal{H}(\rho_h^\gamma), \pi_h((G_\delta^L)'(\rho_h^\gamma)))) \geq \frac{1}{\Delta t} \left(\frac{\gamma^2}{4L} - C(L)|\Omega| \right) - \frac{1}{\Delta t} \int_{\Omega} \pi_h(G_\delta^L(\rho_h^{n-1})) \, dx.$$

Thus, for $\gamma > [4L(C(L)|\Omega| + \|\pi_h(G_\delta^L(\rho_h^{n-1}))\|_{L^1(\Omega)})]^{1/2}$ we have

$$((\mathcal{H}(\rho_h^\gamma), \pi_h((G_\delta^L)'(\rho_h^\gamma)))) > 0,$$

and hence we have arrived at a contradiction; therefore the function $\mathcal{H}$ has a zero, which means that at time t_n there exists a solution $\rho_{h,\delta,L}^n \in V_h$ to the fully discrete scheme (1.27a). Having shown the existence of $\rho_{h,\delta,L}^n \in V_h$, the existence of an associated (unique) $c_{h,\delta,L}^n \in V_h \cap L_*^2(\Omega)$ follows from (1.27b). $\square$

We need a series of additional results before proceeding to the proof of convergence as δ and h tend to zero.

Lemma 1.12. *A solution $\{\rho_{h,\delta,L}^n\}_{n=1}^N \subset V_h$ of (1.27a) satisfies the following bound:*

$$\max_{n=1,\dots,N} \int_{\Omega} (\rho_{h,\delta,L}^n)^2 \, dx + \frac{1}{\delta} \max_{n=1,\dots,N} \int_{\Omega} \pi_h([\rho_{h,\delta,L}^n]_-^2) \, dx + \Delta t \sum_{n=1}^N \int_{\Omega} |\nabla \rho_{h,\delta,L}^n|^2 \, dx \leq C(L). \quad (1.35)$$

Proof. We sum the bounds (1.31) over $n = 1, \dots, m$ to deduce that, for each $m \in \{1, \dots, N\}$,

$$\int_{\Omega} \pi_h(G_\delta^L(\rho_{h,\delta,L}^m)) \, dx + \Delta t \sum_{n=1}^m \int_{\Omega} \nabla \rho_{h,\delta,L}^n \cdot \nabla \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) \, dx \leq \int_{\Omega} \pi_h(G_\delta^L(\rho_h^0)) \, dx.$$

Using Corollary 1.9 with $\phi_h = \rho_{h,\delta,L}^n$ and $g = (G_\delta^L)'$, noting that g is strictly monotonically increasing and the inverse g^{-1} is Lipschitz continuous with Lipschitz constant L , we then have that, for each $m \in \{1, \dots, N\}$,

$$\int_{\Omega} \pi_h(G_\delta^L(\rho_{h,\delta,L}^m)) \, dx + \frac{\Delta t}{L} \sum_{n=1}^m \int_{\Omega} |\nabla \rho_{h,\delta,L}^n|^2 \, dx \leq \int_{\Omega} \pi_h(G_\delta^L(\rho_h^0)) \, dx.$$

Let $\Omega_+ := \{x \in \bar{\Omega} : \rho_{h,\delta,L}^n \geq 0\}$ and let $\Omega_- := \bar{\Omega} \setminus \Omega_+$. We shall further bound the first term on the left-hand side of this inequality from below by noting that, thanks to (1.15) and (1.23), we have

$$\begin{aligned} \int_{\Omega} \pi_h(G_\delta^L(\rho_{h,\delta,L}^n)) \, dx &= \int_{\Omega_+} \pi_h(G_\delta^L(\rho_{h,\delta,L}^n)) \, dx + \int_{\Omega_-} \pi_h(G_\delta^L(\rho_{h,\delta,L}^n)) \, dx \\ &\geq \frac{1}{4L} \int_{\Omega_+} \pi_h((\rho_{h,\delta,L}^n)^2) \, dx - C(L)|\Omega_+| + \frac{1}{2\delta} \int_{\Omega_-} \pi_h((\rho_{h,\delta,L}^n)^2) \, dx \\ &= \frac{1}{4L} \int_{\Omega} \pi_h((\rho_{h,\delta,L}^n)^2) \, dx - C(L)|\Omega_+| + \frac{1}{2\delta} \int_{\Omega_-} \pi_h((\rho_{h,\delta,L}^n)^2) \, dx \\ &\quad - \frac{1}{4L} \int_{\Omega_-} \pi_h((\rho_{h,\delta,L}^n)^2) \, dx \\ &\geq \frac{1}{4L} \int_{\Omega} (\pi_h \rho_{h,\delta,L}^n)^2 \, dx + \frac{1}{4\delta} \int_{\Omega} \pi_h([\rho_{h,\delta,L}^n]_-^2) \, dx - C(L)|\Omega| \\ &= \frac{1}{4L} \int_{\Omega} (\rho_{h,\delta,L}^n)^2 \, dx + \frac{1}{4\delta} \int_{\Omega} \pi_h([\rho_{h,\delta,L}^n]_-^2) \, dx - C(L)|\Omega|, \end{aligned}$$

where in the transition to the fourth line we have used that $\delta < L$ and that $[\rho_{h,\delta,L}^n]_-^2 \equiv 0$ on Ω_+ . It remains to note that, because for all δ and L such that $0 < \delta < 1 < L$ we have that

$$0 \leq G_\delta^L(r) \leq \max \left\{ 1 - \frac{\delta}{2}, G_\delta^L(M) \right\}, \quad \text{for all } r \in [0, M],$$

and, assuming without loss of generality that $L > \|\rho_0\|_{L^\infty(\Omega)}$, it follows from (1.26) that $0 \leq G_\delta^L(\rho_{h,\delta,L}^0) \leq C$, where $C = C(L)$ is a positive constant, independent of h and δ , whereby the same is true of $\int_{\Omega} \pi_h(G_\delta^L(\rho_{h,\delta,L}^0)) \, dx$. As Ω is a fixed domain, we shall absorb $|\Omega|$ into $C(L)$ and write $C(L)$ instead of $C(L)|\Omega|$. From this, the inequality (1.35) directly follows. $\square$

The final piece of information we need before taking the limit concerns the convergence of the discrete fractional Laplacian $(-\Delta_h)^s$ and thus of the solution $c_{h,\delta,L}^n$ of the finite-dimensional fractional Poisson problem. We will rely on the results that were proved in [39, 43, 44], where fractional powers of elliptic operators and their finite element approximation were studied in the setting that we have put in place.

Proposition 1.13 (Convergence of the spatial discretization of the fractional Laplacian). *Suppose that $s \in (0, 1)$, $\sigma \in [0, 1]$ and $f \in \mathbb{H}_*^{2\sigma}(\Omega)$. Then, there exists a positive constant C that is independent of h , σ and f such that*

$$\|(-\Delta_N)^{-s} f - (-\Delta_h)^{-s} \Pi_h f\|_{L^2(\Omega)} \leq C\varepsilon(h) \|f\|_{\mathbb{H}_*^{2\sigma}(\Omega)} \quad \text{for all } f \in \mathbb{H}_*^{2\sigma}(\Omega),$$

where

$$\varepsilon(h) = \begin{cases} h^2 & \text{if } s + \sigma > 1, \\ \log(h^{-1})h^2 & \text{if } s + \sigma = 1, \\ \log(h^{-1})h^{2(s+\sigma)} & \text{if } s + \sigma < 1, \end{cases}$$

and Π_h is the $L^2(\Omega)$ projection into the linear space V_h .

Now we are ready for passage to the limit with $\delta \rightarrow 0_+$ and $h \rightarrow 0_+$. As we said previously, passage to the limit $\Delta t \rightarrow 0_+$ will be discussed in the next section. It will be also shown that by taking $L > \|\rho_0\|_{L^\infty(\Omega)}$ the sequence of numerical solutions becomes independent of L , so passage to the limit $L \rightarrow +\infty$ is not required.

Theorem 1.14. *The initial data $\{\rho_h^0\}_{h>0}$ defined in (1.24) are such that, for Δt and L fixed, as $h \rightarrow 0_+$ we have that*

$$\rho_h^0 \rightarrow \rho_L^0 = \rho^0 := \rho^0(\Delta t) \quad \text{strongly in } L^2(\Omega). \quad (1.36)$$

Furthermore there exists a subsequence of $\{\rho_{h,\delta,L}^n\}_{\delta,h>0}$, a nonnegative function $\rho_L^n \in V = H^1(\Omega)$ and $c_L^n \in H_*^1(\Omega)$ such that the following convergence results hold, for each $n \in \{1, \dots, N\}$, as $\delta, h \rightarrow 0_+$:

$$\nabla \rho_{h,\delta,L} \rightarrow \nabla \rho_L^n \quad \text{weakly in } L^2(\Omega; \mathbb{R}^d), \quad (1.37a)$$

$$\rho_{h,\delta,L}^n \rightarrow \rho_L^n \quad \text{strongly in } L^2(\Omega), \quad (1.37b)$$

$$\Theta_\delta^L(\rho_{h,\delta,L}^n) \rightarrow \beta^L(\rho_L^n)I \quad \text{strongly in } L^2(\Omega; \mathbb{R}^{d \times d}), \quad (1.37c)$$

$$c_{h,\delta,L}^n \rightarrow c_L^n \quad \text{strongly in } L_*^2(\Omega), \quad (1.37d)$$

$$\nabla c_{h,\delta,L}^n \rightarrow \nabla c_L^n \quad \text{weakly in } L_*^2(\Omega; \mathbb{R}^d). \quad (1.37e)$$

Moreover $\{\rho_L^n\}_{n=1,\dots,N}$ solves the problem (1.30a), $\rho_L^n \geq 0$ a.e. on Ω for all $n = 1, \dots, N$, and, given $\rho_L^0 = \rho^0$ such that $\frac{1}{|\Omega|} \int_\Omega \rho^0 dx = 1$, one has $\frac{1}{|\Omega|} \int_\Omega \rho_L^n dx = 1$ for all $n = 1, \dots, N$.

Proof. It follows from (1.25) that there exists a subsequence of $\{\rho_h^0\}_{h>0}$ (which, for the sake of simplicity of notation, we shall continue to denote by $\{\rho_h^0\}_{h>0}$) that converges weakly in $L^2(\Omega)$ to some element $g \in L^2(\Omega)$, and $\nabla \rho_h^0$ converges weakly to some element $G \in L^2(\Omega; \mathbb{R}^d)$, as $h \rightarrow 0_+$. To show that $G = \nabla g$ notice that for any $\eta \in C_0^\infty(\Omega; \mathbb{R}^d)$ we have

$$\int_\Omega G \cdot \eta dx \leftarrow \int_\Omega \nabla \rho_h^0 \cdot \eta dx = - \int_\Omega \rho_h^0 \operatorname{div} \eta dx \rightarrow - \int_\Omega g \operatorname{div} \eta dx,$$

which means that G is the distributional gradient of g , i.e., $G = \nabla g$ in $(C_0^\infty(\Omega; \mathbb{R}^d))'$, but since $G \in L^2(\Omega; \mathbb{R}^d)$ we then have that $G = \nabla g \in L^2(\Omega; \mathbb{R}^d)$. The compact embedding $H^1(\Omega) \hookrightarrow L^2(\Omega)$ implies that (a subsequence of) $\{\rho_h^0\}_{h>0}$ converges strongly in $L^2(\Omega)$ to $g \in L^2(\Omega)$ as $h \rightarrow 0_+$, and therefore we can pass to the limit in (1.24) with $\phi_h = \pi_h \phi$ for any function $\phi \in C^\infty(\overline{\Omega})$ to get equation (1.28). This shows that $g = \rho^0$, and the fact that $C^\infty(\overline{\Omega})$ is dense in $V = H^1(\Omega)$ then implies (1.36).

Now, let $n \in \{1, \dots, N\}$. The weak convergence (1.37a) and the strong convergence (1.37b) are implied by the inequality (1.35) and the same considerations as the ones we exposed above in the case of $\nabla \rho_h^0$ and ρ_0^h . The nonnegativity of the limit function ρ_L^n follows from (1.37b) and the second bound in (1.35).

Combining the second and third bounds in (1.35) and Lemma 1.7 we have the result (1.37c).

The convergence result (1.37d) can be proved in the following way. We have, by use of the stability inequality (A.3) satisfied by the solution of the fractional Poisson equation, that

$$\begin{aligned} & \|(-\Delta_N)^{-s}(\rho_L^n)^* - (-\Delta_h)^{-s}(\rho_{h,\delta,L}^n)^*\|_{L^2(\Omega)} \\ & \leq \|(-\Delta_N)^{-s}((\rho_L^n)^* - (\rho_{h,\delta,L}^n)^*)\|_{L^2(\Omega)} + \|((-\Delta_N)^{-s} - (-\Delta_h)^{-s})(\rho_{h,\delta,L}^n)^*\|_{L^2(\Omega)} \\ & \leq C\|(\rho_L^n)^* - (\rho_{h,\delta,L}^n)^*\|_{L^2(\Omega)} + \|((-\Delta_N)^{-s} - (-\Delta_h)^{-s})(\rho_{h,\delta,L}^n)^*\|_{L^2(\Omega)}, \end{aligned}$$

and by (1.37b) and the convergence result stated in Proposition 1.13 we have (1.37d); here and henceforth C signifies a generic positive constant, independent of δ and h .

To prove (1.37e) we need a uniform bound on the gradient of $c_{h,\delta,L}^n$; then, the result will follow from (1.37d). Thanks to [98, Theorem 4.8.12] we have that

$$\|(I - \mathcal{S}_h)v\|_{L^2(\Omega)} + h|(I - \mathcal{S}_h)v|_{H^1(\Omega)} \leq Ch|v|_{H^1(\Omega)} \quad \text{for all } v \in H^1(\Omega), \quad (1.38)$$

where $\mathcal{S}_h$ denotes the Scott–Zhang quasi-interpolation operator. For any $v_h \in V_h$, thanks to the assumed quasi-uniformity of the family of triangulations, we have also

$$\|\nabla v_h\|_{L^2(\Omega)} \leq Ch^{-1}\|v_h\|_{L^2(\Omega)}. \quad (1.39)$$

Let us denote by $\tilde{c}_{h,\delta,L}^n \in H_*^1(\Omega)$ the solution of the auxiliary boundary-value problem

$$-(-\Delta_N)^s \tilde{c}_{h,\delta,L}^n = (\rho_{h,\delta,L}^n)^* \quad \text{in } \Omega.$$

Then, the gradient of $c_{h,\delta,L}^n$ satisfies the following chain of inequalities:

$$\begin{aligned} \|\nabla c_{h,\delta,L}^n\|_{L^2(\Omega)} & \leq \|\nabla(c_{h,\delta,L}^n - \mathcal{S}_h \tilde{c}_{h,\delta,L}^n)\|_{L^2(\Omega)} + \|\nabla(\mathcal{S}_h \tilde{c}_{h,\delta,L}^n - \tilde{c}_{h,\delta,L}^n)\|_{L^2(\Omega)} + \|\nabla \tilde{c}_{h,\delta,L}^n\|_{L^2(\Omega)} \\ & \leq \frac{C}{h}\|c_{h,\delta,L}^n - \mathcal{S}_h \tilde{c}_{h,\delta,L}^n\|_{L^2(\Omega)} + C\|\nabla \tilde{c}_{h,\delta,L}^n\|_{L^2(\Omega)} \\ & \leq \frac{C}{h}\|c_{h,\delta,L}^n - \tilde{c}_{h,\delta,L}^n\|_{L^2(\Omega)} + \frac{C}{h}\|\tilde{c}_{h,\delta,L}^n - \mathcal{S}_h \tilde{c}_{h,\delta,L}^n\|_{L^2(\Omega)} + C\|\nabla \tilde{c}_{h,\delta,L}^n\|_{L^2(\Omega)}, \end{aligned}$$

where in the transition from the first to the second line we used (1.39) to bound the first term on the right-hand side of the first line, and (1.38) to bound the second term on the right-hand side of the first line. Because $c_{h,\delta,L}^n = -(-\Delta_h)^{-s}(\rho_{h,\delta,L}^n)^*$ and $\tilde{c}_{h,\delta,L}^n = -(-\Delta_N)^{-s}(\rho_{h,\delta,L}^n)^*$, the first term in the last line is now uniformly bounded thanks to Proposition 1.13 with $\sigma = 1/2$ and $\varepsilon(h) = \ln(h^{-1})h^{2s+1}$ if $s < \frac{1}{2}$, $\varepsilon(h) = h^2$ if $s > \frac{1}{2}$, $\varepsilon(h) = \ln(h^{-1})h^2$ if $s = \frac{1}{2}$, and the fact that $(\rho_{h,\delta,L}^n)^* := \rho_{h,\delta,L}^n - \int_\Omega \rho_{h,\delta,L}^n dx \in V_h$ is uniformly bounded in $H_*^{2\sigma}(\Omega) = H_*^1(\Omega)$ as $h, \delta \rightarrow 0_+$ because of (1.35). The second term in the last line is uniformly bounded by the interpolation

inequality (1.38), (A.5) in Lemma A.6 and the bound on the third term on the left-hand side of (1.35). For the third term in the last line, we have similarly, thanks to (A.5), that

$$\|\nabla \tilde{c}_{h,\delta,L}^n\|_{L^2(\Omega)} \leq C \|\nabla \rho_{h,\delta,L}^n\|_{L^2(\Omega)}$$

and the bound on the third term on the left-hand side of (1.35) then makes the term uniformly bounded with respect to h and δ . Having shown that $\nabla c_{h,\delta,L}^n$ is uniformly bounded in $L^2(\Omega; \mathbb{R}^d)$ as $h, \delta \rightarrow 0_+$, the weak convergence result (1.37e) follows from (1.37d) thanks to the uniqueness of the weak limit.

We combine (1.37a)–(1.37c) to pass to the limit as $\delta, h \rightarrow 0_+$ in (1.27a) with $\phi_h = \pi_h \phi$, for $\phi \in C^\infty(\bar{\Omega})$ together with the strong convergence of $\pi_h \phi$ to ϕ in the norm of $W^{1,\infty}(\Omega)$ as $h \rightarrow 0_+$ (cf., for example, inequality (4.4.29) in [49] with $s = 1$, $m = 2$, $l = 1$, $r = 0$ and $p = \infty$ there), to obtain equation (1.30a). The fact that $C^\infty(\bar{\Omega})$ is dense in $V = H^1(\Omega)$ then concludes the argument. The nonnegativity of $\rho_{h,\delta,L}^n$ on $\bar{\Omega}$ implies the nonnegativity of ρ_L^n a.e. on Ω for $n = 1, \dots, N$. Finally, we note that if we choose $\phi \equiv 1$ as a test function in (1.30a) we have conservation of mass, i.e., $\frac{1}{|\Omega|} \int_{\Omega} \rho_L^n(x) dx = \frac{1}{|\Omega|} \int_{\Omega} \rho^0 dx = 1$ for ρ_L^n , $n = 1, \dots, N$. $\square$

Remark 1.15. The proof of Theorem 1.14 allows us to further motivate our choice to employ the spectral fractional Laplacian in our analysis. A careful look at the proof of the theorem shows that, in order to prove the convergence of the potential $c_{h,\delta,L}^n$ (1.37d) for any $s \in (0, 1)$, we have demanded a superlinear convergence rate in $L^2(\Omega)$, provided by Proposition 1.13, having $H^1(\Omega)$ regularity of the right-hand side datum. This contrasts (sub)linear convergence rates of the integral fractional Laplacian, that were proved for classical FE schemes for the Dirichlet problem [5] and observed also for the Neumann problem [28].

Having passed to the limits $h \rightarrow 0_+$ and $\delta \rightarrow 0_+$ with the spatial discretization parameter h and the lower cut-off parameter δ , in the next section we shall focus on passage to the limits $\Delta t \rightarrow 0_+$ and $L \rightarrow +\infty$ with the time step Δt and the upper cut-off parameter L .

1.3 The semidiscrete-in-time approximation

Next, we shall pass to the limit as the time-step $\Delta t > 0$ tends to zero in the temporally semidiscrete scheme (1.30), which we presented in the previous section, and which we obtained as the limit of the finite element approximation when $\delta, h \rightarrow 0_+$, as was shown in Theorem 1.14.

In order to pass to the limit $\Delta t \rightarrow 0_+$ we shall first show that the approximation is independent of the cut-off parameter L , provided that $L > \|\rho_0\|_{L^\infty(\Omega)}$; we shall then derive uniform bounds with respect to Δt and proceed by extraction of weakly convergent subsequences as $\Delta t \rightarrow 0_+$, similarly as we did in the previous section in the case of the parameters δ and h .

Suppose that $N \in \mathbb{N}_{\geq 2}$ and $\Delta t := T/N$. We then define

$$\rho_L^{\Delta t}(\cdot, t) := \frac{t - t_{n-1}}{\Delta t} \rho_L^n(\cdot) + \frac{t_n - t}{\Delta t} \rho_L^{n-1}(\cdot), \quad t \in [t_{n-1}, t_n], \quad n = 1, \dots, N, \quad (1.40a)$$

that is, the continuous piecewise affine interpolant in time of the sequence of discrete-in-time approximations $\{\rho_L^n\}_{n=1,\dots,N}$, in conjunction with the notation

$$\rho_L^{\Delta t,+}(\cdot, t) := \rho_L^n(\cdot), \quad \rho_L^{\Delta t,-}(\cdot, t) := \rho_L^{n-1}(\cdot), \quad t \in (t_{n-1}, t_n], \quad n = 1, \dots, N. \quad (1.40b)$$

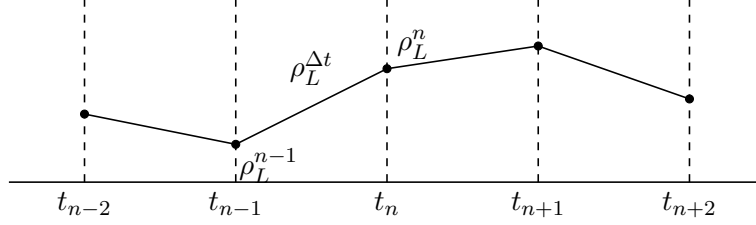


Figure 1.2: Continuous piecewise affine interpolant of the discrete-in-time approximations

We shall adopt $\rho_L^{\Delta t(\pm)}$ as a collective symbol for $\rho_L^{\Delta t}, \rho_L^{\Delta t,\pm}$. For future purposes we observe that

$$\frac{\partial \rho_L^{\Delta t}}{\partial t}(\cdot, t) = \frac{\rho_L^{\Delta t,+}(\cdot, t) - \rho_L^{\Delta t,-}(\cdot, t)}{\Delta t}, \quad t \in (t_{n-1}, t_n], \quad n = 1, \dots, N,$$

and that, thanks to the final assertion in Theorem 1.14, one has that

$$\frac{1}{|\Omega|} \int_{\Omega} \rho_L^{\Delta t(\pm)}(t) \, dx = \frac{1}{|\Omega|} \int_{\Omega} \rho^0 \, dx = 1, \quad t \in (t_{n-1}, t_n], \quad n = 1, \dots, N.$$

For $t \in (0, T]$, let $c_L^{\Delta t}(\cdot, t) \in \mathbb{H}^s(\Omega) \cap H_*^1(\Omega)$ be the unique solution of the equation

$$-(-\Delta_N)^s c_L^{\Delta t} = (\rho_L^{\Delta t})^* \quad \text{in } \Omega. \quad (1.41)$$

We note in passing that, thanks to linearity and because $\frac{1}{|\Omega|} \int_{\Omega} \rho_L^n \, dx = \frac{1}{|\Omega|} \int_{\Omega} \rho_L^0 \, dx = \frac{1}{|\Omega|} \int_{\Omega} \rho_0 \, dx = 1$ for all $n = 1, \dots, N$, we have that

$$(\rho_L^{\Delta t})^*(\cdot, t) := \rho_L^{\Delta t} - \frac{1}{|\Omega|} \int_{\Omega} \rho_L^{\Delta t} \, dx = \frac{t - t_{n-1}}{\Delta t} (\rho_L^n)^*(\cdot) + \frac{t_n - t}{\Delta t} (\rho_L^{n-1})^*(\cdot),$$

for $t \in [t_{n-1}, t_n]$, $n = 1 \dots, N$, and therefore

$$\frac{\partial (\rho_L^{\Delta t})^*}{\partial t}(\cdot, t) = \frac{(\rho_L^{\Delta t,+})^*(\cdot, t) - (\rho_L^{\Delta t,-})^*(\cdot, t)}{\Delta t} = \frac{\partial \rho_L^{\Delta t}}{\partial t}(\cdot, t), \quad (1.42)$$

for $t \in [t_{n-1}, t_n]$, $n = 1 \dots, N$.

Using the above notation, (1.30a) summed through $n = 1, \dots, N$, can be restated in a form that is reminiscent of a weak formulation in time, that is:

$$\begin{aligned} & \text{Find } \rho_L^{\Delta t}(\cdot, t) \in V = H^1(\Omega) \text{ for } t \in (0, T], \text{ such that} \\ & \int_0^T \int_{\Omega} \frac{\partial \rho_L^{\Delta t}}{\partial t} \phi \, dx \, dt = - \int_0^T \int_{\Omega} \nabla \rho_L^{\Delta t,+} \cdot \nabla \phi \, dx \, dt + \int_0^T \int_{\Omega} \beta^L(\rho_L^{\Delta t,+}) \nabla c_L^{\Delta t,+} \cdot \nabla \phi \, dx \, dt \\ & \text{for all } \phi \in L^1(0, T; V), \end{aligned} \quad (1.43a)$$

subject to the initial condition $\rho_L^{\Delta t}(x, 0) = \rho^0(x)$ for a.e. $x \in \Omega$, where $c_L^{\Delta t, +}(\cdot, t) \in H_*^1(\Omega)$ for all $t \in (0, T]$ and satisfies

$$-(-\Delta_N)^s c_L^{\Delta t, +}(\cdot, t) = (\rho_L^{\Delta t, +})^*(\cdot, t) \quad \text{in } \Omega, \quad (1.43b)$$

for all $t \in (0, T]$, and $\beta^L(r) := \min\{r, L\}$ for $r \in \mathbb{R}_{\geq 0}$.

We shall now rigorously prove a result similar to the one that we obtained through formal calculations for smooth solutions in Lemma 1.1, namely a uniform bound in time on the $L^\infty(\Omega)$ norm of the solution $\rho_L^{\Delta t}$. This property will allow us to eliminate the parameter L . Moreover the bound will be decisive in the convergence argument that follows, and it is the place where the structure of the problem and the action of the fractional Laplacian proves advantageous. As was noted previously, in [71] this result was shown for a smooth solution of the continuous model on the whole of $\mathbb{R}^d$ using the integral definition of the fractional Laplacian, while in Lemma 1.1 above it was asserted for a bounded domain using the spectral definition of the fractional Neumann Laplacian, based on formal calculations. Our starting point is the following lemma.

Lemma 1.16. *Let $\rho_L^{\Delta t, +}$ be defined as in (1.40) and let $F \in C^2([0, \infty))$ be a convex and non-decreasing function. Then,*

$$\sup_{t \in (0, T]} \int_{\Omega} F(\rho_L^{\Delta t, +}(t)) \, dx \leq \int_{\Omega} F(\rho^0) \, dx. \quad (1.44)$$

Proof. We begin by noting that, because $\rho^0 \in L^\infty(\Omega)$, we have that $F(\rho^0) \in L^1(\Omega)$, and the right-hand side of the inequality (1.44) is therefore finite. Let us assume first that F'' is additionally bounded (for the general case one can use a similar argument as the one in the end of the proof of Lemma 1.1). Let us then pick $\phi = \chi_{[0, t]} F'(\rho_L^{\Delta t, +})$ with $t = t_n$ for $n = 1, \dots, N$, as test function in (1.43a). We then have that

$$\begin{aligned} \int_0^{t_n} \int_{\Omega} \frac{\partial \rho_L^{\Delta t}}{\partial t} F'(\rho_L^{\Delta t, +}) \, dx \, d\tau &= - \int_0^{t_n} \int_{\Omega} F''(\rho_L^{\Delta t, +}) |\nabla \rho_L^{\Delta t, +}|^2 \, dx \, d\tau \\ &\quad + \int_0^{t_n} \int_{\Omega} \beta^L(\rho_L^{\Delta t, +}) F''(\rho_L^{\Delta t, +}) \nabla c_L^{\Delta t, +} \cdot \nabla \rho_L^{\Delta t, +} \, dx \, d\tau. \end{aligned} \quad (1.45)$$

The first term on the right-hand side is always nonpositive thanks to the convexity of F . For the second term on the right-hand side we can write

$$\begin{aligned} &\int_0^{t_n} \int_{\Omega} \beta^L(\rho_L^{\Delta t, +}) F''(\rho_L^{\Delta t, +}) \nabla c_L^{\Delta t, +} \cdot \nabla \rho_L^{\Delta t, +} \, dx \, d\tau \\ &= - \int_0^{t_n} \int_{\Omega} \beta^L(\rho_L^{\Delta t, +}) F''(\rho_L^{\Delta t, +}) \nabla \rho_L^{\Delta t, +} \cdot \nabla (-\Delta_N)^{-s} (\rho_L^{\Delta t, +})^* \, dx \, d\tau \\ &= - \int_0^{t_n} \int_{\Omega} \nabla H(\rho_L^{\Delta t, +}) \cdot \nabla (-\Delta_N)^{-s} (\rho_L^{\Delta t, +})^* \, dx \, d\tau, \end{aligned} \quad (1.46)$$

where $H(r) := \int_0^r \beta^L(\tau) F''(\tau) \, d\tau$ is a nondecreasing function by definition.

We want to employ an argument similar to the one we used in Lemma 1.1 to show that the minus sign on the left-hand side of the fractional Poisson equation (1.43b) and the explicit representation of the spectral fractional Neumann Laplacian in terms of the heat kernel guarantee nonpositivity of the expression in the last line of (1.46) above, but in order to rigorously replicate the formal argument of Lemma 1.1 we require additional considerations. We would like to perform spatial integration by parts, as we did in (1.8), to prove the nonpositivity of the term (1.46); but now $\rho_L^{\Delta t, +} \in L^\infty(0, T; H^1(\Omega))$ only, so we cannot proceed directly. We shall therefore consider a sequence of functions $\{\rho_{L, \epsilon}^{\Delta t, +}\}_{\epsilon > 0} \subset L^\infty(0, T; C^\infty(\bar{\Omega}))$, such that $\rho_{L, \epsilon}^{\Delta t, +} \rightarrow \rho_L^{\Delta t, +}$ strongly in $L^2(0, T; H^1(\Omega))$ as $\epsilon \rightarrow 0_+$ and $\rho_{L, \epsilon}^{\Delta t, +} \geq 0$ for a.e. $(x, t) \in \Omega \times (0, T]$. Such a sequence of smooth functions exists thanks to the density of $C^\infty(\bar{\Omega})$ in $H^1(\Omega)$, and is easily constructed by extending $\rho_L^{\Delta t, +}(\cdot, t) \geq 0$ from Ω to the whole of $\mathbb{R}^d$ by preserving the Sobolev class $H^1(\Omega)$, and convolving the nonnegative part of the extended function with $\theta_\epsilon(x) = \epsilon^{-d}\theta(x/\epsilon)$, where $\theta \in C_0^\infty(\mathbb{R}^d)$ is a nonnegative function such that $\int_{\mathbb{R}^d} \theta(x) dx = 1$. Instead of the right-hand side of (1.46) we shall then consider the term

$$\textcircled{\dagger} = - \int_0^{t_n} \int_\Omega \nabla H(\rho_{L, \epsilon}^{\Delta t, +}) \cdot \nabla (-\Delta_N)^{-s} (\rho_{L, \epsilon}^{\Delta t, +})^* dx d\tau.$$

Proceeding in the same way as we did in Lemma 1.1, using integration by parts, we have that

$$\textcircled{\dagger} = - \int_0^{t_n} \int_\Omega H(\rho_{L, \epsilon}^{\Delta t, +}) (-\Delta_N)^{1-s} (\rho_{L, \epsilon}^{\Delta t, +})^* dx d\tau, \quad (1.47)$$

and then the nonpositivity of the expression above follows from the same argument as in the case of the second term in (1.8) in the proof of Lemma 1.1.

To prove the nonpositivity of the right-hand side of (1.46) it remains to show that, as $\epsilon \rightarrow 0_+$,

$$\textcircled{\dagger} \rightarrow - \int_0^{t_n} \int_\Omega \nabla H(\rho_L^{\Delta t, +}) \cdot \nabla (-\Delta_N)^{-s} (\rho_L^{\Delta t, +})^* dx d\tau. \quad (1.48)$$

To see this, we observe that

$$\begin{aligned} & \int_0^{t_n} \int_\Omega (\nabla H(\rho_{L, \epsilon}^{\Delta t, +}) \cdot \nabla (-\Delta_N)^{-s} (\rho_{L, \epsilon}^{\Delta t, +})^* - \nabla H(\rho_L^{\Delta t, +}) \cdot \nabla (-\Delta_N)^{-s} (\rho_L^{\Delta t, +})^*) dx d\tau \\ &= \underbrace{\int_0^{t_n} \int_\Omega (\nabla H(\rho_{L, \epsilon}^{\Delta t, +}) - \nabla H(\rho_L^{\Delta t, +})) \cdot \nabla (-\Delta_N)^{-s} (\rho_{L, \epsilon}^{\Delta t, +})^* dx d\tau}_{\textcircled{1}} \\ &+ \underbrace{\int_0^{t_n} \int_\Omega \nabla H(\rho_L^{\Delta t, +}) \cdot \nabla (-\Delta_N)^{-s} ((\rho_{L, \epsilon}^{\Delta t, +})^* - (\rho_L^{\Delta t, +})^*) dx d\tau}_{\textcircled{2}}. \end{aligned}$$

Term $\textcircled{2}$ converges to zero as $\epsilon \rightarrow 0_+$, because the function $\nabla H(\rho_L^{\Delta t, +})$ which is equal to $\beta^L(\rho_L^{\Delta t, +})F''(\rho_L^{\Delta t, +})\nabla \rho_L^{\Delta t, +}$ belongs to $L^\infty(0, T; L^2(\Omega; \mathbb{R}^d))$ (recall that β^L is a bounded

function by definition, and F'' is a bounded function by assumption), and because for each $\eta \in L^\infty(0, T; C_0^\infty(\Omega; \mathbb{R}^d))$ we have that

$$\begin{aligned} \left| \int_0^{t_n} (\eta, \nabla(-\Delta)^{-s}((\rho_{L,\epsilon}^{\Delta t,+})^* - (\rho_L^{\Delta t,+})^*)) dt \right| &= \left| \int_0^{t_n} (\operatorname{div} \eta, (-\Delta_N)^{-s}((\rho_{L,\epsilon}^{\Delta t,+})^* - (\rho_L^{\Delta t,+})^*)) dt \right| \\ &= \left| \int_0^{t_n} ((-\Delta_N)^{-s} \operatorname{div} \eta, (\rho_{L,\epsilon}^{\Delta t,+})^* - (\rho_L^{\Delta t,+})^*) dt \right| \\ &\leq \|(-\Delta_N)^{-s} \operatorname{div} \eta\|_{L^2(0,T;L^2(\Omega))} \|(\rho_{L,\epsilon}^{\Delta t,+})^* - (\rho_L^{\Delta t,+})^*\|_{L^2(0,T;L^2(\Omega))} \rightarrow 0 \end{aligned}$$

as $\epsilon \rightarrow 0_+$. We note in passing that $\int_\Omega \operatorname{div} \eta(x, t) dx = \int_{\partial\Omega} \eta(x, t) \cdot n ds = 0$, whereby $\operatorname{div} \eta(\cdot, t) \in L_*^2(\Omega)$ for a.e. $t \in (0, T]$ and $(-\Delta_N)^{-s} \operatorname{div} \eta(\cdot, t)$ therefore belongs to $L_*^2(\Omega)$ for all $s \in (0, 1)$, and for a.e. $t \in (0, T]$. Thanks to the fact that $C_0^\infty(\Omega; \mathbb{R}^d)$ is dense in $L^2(\Omega; \mathbb{R}^d)$ it follows that

$$\int_0^{t_n} (\eta, \nabla(-\Delta_N)^{-s}((\rho_{L,\epsilon}^{\Delta t,+})^* - (\rho_L^{\Delta t,+})^*)) dt \rightarrow 0$$

as $\epsilon \rightarrow 0_+$ for all $\eta \in L^\infty(0, T; L^2(\Omega; \mathbb{R}^d))$, so in particular this is true for

$$\eta = \beta^L(\rho_L^{\Delta t,+}) F''(\rho_L^{\Delta t,+}) \nabla \rho_L^{\Delta t,+} = \nabla H(\rho_L^{\Delta t,+}) \in L^\infty(0, T; L^2(\Omega; \mathbb{R}^d)).$$

Thus we have shown that the term ② converges to 0 as $\epsilon \rightarrow 0_+$.

For term ① we have that

$$\begin{aligned} |\textcircled{1}| &= \left| \int_0^{t_n} \int_\Omega (\beta^L(\rho_{L,\epsilon}^{\Delta t,+}) F''(\rho_{L,\epsilon}^{\Delta t,+}) \nabla \rho_{L,\epsilon}^{\Delta t,+} - \beta^L(\rho_L^{\Delta t,+}) F''(\rho_L^{\Delta t,+}) \nabla \rho_L^{\Delta t,+}) \right. \\ &\quad \left. \cdot \nabla(-\Delta_N)^{-s}(\rho_{L,\epsilon}^{\Delta t,+})^* dx d\tau \right| \\ &\leq \|\beta^L(\rho_{L,\epsilon}^{\Delta t,+}) F''(\rho_{L,\epsilon}^{\Delta t,+}) \nabla \rho_{L,\epsilon}^{\Delta t,+} - \beta^L(\rho_L^{\Delta t,+}) F''(\rho_L^{\Delta t,+}) \nabla \rho_L^{\Delta t,+}\|_{L^2(0,T;L^2(\Omega))} \\ &\quad \times \|\nabla(-\Delta_N)^{-s}(\rho_{L,\epsilon}^{\Delta t,+})^*\|_{L^2(0,T;L^2(\Omega))}. \end{aligned}$$

Focusing on the first factor on the right-hand side of the last inequality, we have that

$$\begin{aligned} &\|\beta^L(\rho_{L,\epsilon}^{\Delta t,+}) F''(\rho_{L,\epsilon}^{\Delta t,+}) \nabla \rho_{L,\epsilon}^{\Delta t,+} - \beta^L(\rho_L^{\Delta t,+}) F''(\rho_L^{\Delta t,+}) \nabla \rho_L^{\Delta t,+}\|_{L^2(0,T;L^2(\Omega))} \\ &\leq \|\beta^L(\rho_{L,\epsilon}^{\Delta t,+}) F''(\rho_{L,\epsilon}^{\Delta t,+}) (\nabla \rho_{L,\epsilon}^{\Delta t,+} - \nabla \rho_L^{\Delta t,+})\|_{L^2(0,T;L^2(\Omega))} \\ &\quad + \|(\beta^L(\rho_{L,\epsilon}^{\Delta t,+}) F''(\rho_{L,\epsilon}^{\Delta t,+}) - \beta^L(\rho_L^{\Delta t,+}) F''(\rho_L^{\Delta t,+})) \nabla \rho_L^{\Delta t,+}\|_{L^2(0,T;L^2(\Omega))}. \end{aligned} \tag{1.49}$$

Let us define the constant $M := \sup_{s \in [0, \infty)} F''(s) \geq 0$ (recall that F has been assumed to be a convex function, with F'' bounded on $[0, \infty)$), the first term on the right-hand side of (1.49) is bounded by $LM \|\nabla \rho_{L,\epsilon}^{\Delta t,+} - \nabla \rho_L^{\Delta t,+}\|_{L^2(0,T;L^2(\Omega))}$, which converges to 0 as $\epsilon \rightarrow 0_+$ thanks to the strong convergence of $\rho_{L,\epsilon}^{\Delta t,+}$ to $\rho_L^{\Delta t,+}$ in $L^2(0, T; H^1(\Omega))$. For the second term on the right-hand side of (1.49), because of the strong convergence of $\rho_{L,\epsilon}^{\Delta t,+}$ to $\rho_L^{\Delta t,+}$ in $L^2(0, T; H^1(\Omega))$ there exists a subsequence (not indicated) such that $\rho_{L,\epsilon}^{\Delta t,+}(x, t) \rightarrow \rho_L^{\Delta t,+}(x, t)$ as $\epsilon \rightarrow 0_+$ for a.e. $(x, t) \in \Omega \times (0, T)$. As β^L and F'' are continuous functions we have also that $\beta^L(\rho_{L,\epsilon}^{\Delta t,+}(x, t)) F''(\rho_{L,\epsilon}^{\Delta t,+}(x, t))$

converges to $\beta^L(\rho_L^{\Delta t,+}(x,t))F''(\rho_L^{\Delta t,+}(x,t))$ for a.e. $(x,t) \in \Omega \times (0,T)$ as $\epsilon \rightarrow 0_+$. Hence, by defining

$$A_\epsilon(x,t) = |(\beta^L(\rho_{L,\epsilon}^{\Delta t,+}(x,t))F''(\rho_{L,\epsilon}^{\Delta t,+}(x,t)) - \beta^L(\rho_L^{\Delta t,+}(x,t))F''(\rho_L^{\Delta t,+}(x,t)))\nabla \rho_L^{\Delta t,+}(x,t)|^2,$$

we have also that $A_\epsilon(x,t) \rightarrow 0_+$ as $\epsilon \rightarrow 0_+$ for a.e. $(x,t) \in \Omega \times (0,T)$. Let us note furthermore that $0 \leq A_\epsilon(x,t) \leq 4L^2M^2|\nabla \rho_L^{\Delta t,+}(x,t)|^2$ and that the function $4L^2M^2|\nabla \rho_L^{\Delta t,+}|^2 \in L^1(\Omega \times (0,T))$. Thus, by Lebesgue's dominated convergence theorem $\int_0^T \int_\Omega A_\epsilon(x,t) dx dt \rightarrow 0_+$ as $\epsilon \rightarrow 0_+$, and consequently the second term on the right-hand side of (1.49) also converges to 0 as $\epsilon \rightarrow 0_+$. Thus we have shown that the term ① converges to 0 as $\epsilon \rightarrow 0_+$, which then completes the proof of (1.48).

By combining (1.47) and (1.48), we have proved that the entire right-hand side of (1.45) is nonpositive. For the term on the left-hand side, by Taylor expansion with a remainder of the function

$$r \in [0, \infty) \mapsto F(r + \alpha) \in [0, \infty),$$

where $\alpha \in [0, \infty)$, we have that, for any $b \in [0, \infty)$,

$$(r - b)F'(r + \alpha) = F(r + \alpha) - F(b + \alpha) + \frac{1}{2}(r - b)^2F''(\theta r + (1 - \theta)b + \alpha),$$

with $\theta \in (0, 1)$. By noting that $t \in [0, T] \mapsto \rho_L^{\Delta t}(\cdot, t)$ is piecewise affine relative to the temporal partition $0 = t_0 < t_1 < \dots < t_N = T$, we have that

$$\begin{aligned} \int_0^{t_n} \int_\Omega \frac{\partial \rho_L^{\Delta t}}{\partial t} F'(\rho_L^{\Delta t,+}) dx d\tau &= \int_\Omega F(\rho_L^{\Delta t,+}(x, t_n)) dx - \int_\Omega F(\rho^0(x)) dx \\ &\quad + \frac{1}{2\Delta t} \int_0^{t_n} \int_\Omega F''(\theta \rho_L^{\Delta t,+} + (1 - \theta)\rho_L^{\Delta t,-})(\rho_L^{\Delta t,+} - \rho_L^{\Delta t,-})^2 dx d\tau. \end{aligned}$$

Because the second derivative of F is nonnegative thanks to the assumed convexity of F , we deduce that

$$\int_\Omega F(\rho_L^{\Delta t,+}(x, t_n)) dx \leq \int_\Omega F(\rho^0(x)) dx \quad \text{for all } n \in \{1, \dots, N\},$$

and therefore, because $\rho_L^{\Delta t,+}(\cdot, t)$ is constant on each interval $(t_{n-1}, t_n]$ for $n \in \{1, \dots, N\}$, the inequality (1.44) directly follows.

The assumption made at the start of the proof that F'' is bounded can be removed as at the end of the proof of Lemma 1.1: i.e., we define $F_k(u) := F(0) + F'(0)u + \int_0^u \int_0^v \min(F''(w), k) dw dv$ for $k > 0$; then, $F_k''(u)$ is bounded and the assertion of the lemma follows from the inequality (1.44) with F replaced by F_k ; we then take the limit $k \rightarrow \infty$ using the monotone convergence theorem. $\square$

By recalling the definitions (1.40) we can write, for $t \in (t_{n-1}, t_n]$, $n = 2, \dots, N$,

$$\int_{\Omega} F(\rho_L^{\Delta t, -}(x, t)) \, dx = \int_{\Omega} F(\rho_L^{\Delta t, +}(x, t - \Delta t)) \, dx,$$

and for $0 =: t_0 < t \leq t_1$ we have $\rho_L^{\Delta t, -}(\cdot, t) = \rho^0(\cdot)$, and therefore we have the same bound (1.44) also for $F(\rho_L^{\Delta t, -})$ with $\sup_{t \in (0, T]}$ replaced by $\sup_{t \in (0, T)}$, and consequently, by the convexity of F , for $F(\rho_L^{\Delta t})$, with $\sup_{t \in (0, T]}$ replaced by $\sup_{t \in [0, T]}$. These results can now be used to obtain a result that is analogous to Lemma 1.2.

Lemma 1.17. *Let $\rho_L^{\Delta t(\pm)}$ be defined as in (1.40). Then, the following bound holds:*

$$\sup_{t \in (0, T)} \|\rho_L^{\Delta t(\pm)}(t)\|_{L^\infty(\Omega)} \leq \|\rho_0\|_{L^\infty(\Omega)}. \quad (1.50)$$

Proof. First notice that if we test (1.28) with $F'(\rho^0)$, where $F \in C^2([0, \infty))$ is a nonnegative convex function, then we have, thanks to the nonnegativity of F'' , that

$$\int_{\Omega} (\rho^0 - \rho_0) F'(\rho^0) \, dx \leq 0, \quad \text{and therefore also} \quad \int_{\Omega} F(\rho^0) \, dx \leq \int_{\Omega} F(\rho_0) \, dx,$$

thanks to the convexity of F . Let us now choose a nonnegative convex function $F \in C^2([0, \infty))$ such that $F(u) = 0$ for $u \leq \|\rho_0\|_{L^\infty(\Omega)}$ and $F(u) > 0$ for $u > \|\rho_0\|_{L^\infty(\Omega)}$. Then,

$$0 \leq \int_{\Omega} F(\rho_L^{\Delta t(\pm)}(x, t)) \, dx \leq \int_{\Omega} F(\rho_0(x)) \, dx = 0 \quad \text{for all } t \in (0, T).$$

Consequently $\rho_L^{\Delta t(\pm)} \leq \|\rho_0\|_{L^\infty(\Omega)}$, which then implies the stated $L^\infty(\Omega)$ norm bound. $\square$

Thanks to the fact that (1.50) provides a uniform bound on the $L^\infty(\Omega)$ norm of $\rho^{\Delta t(\pm)}$ for all $t \in (0, T)$, dependent only on the $L^\infty(\Omega)$ norm of the initial datum, the temporally semidiscrete weak formulation (1.43), which we obtained by passing to the limits $h, \delta \rightarrow 0_+$, can be simplified: by assuming without loss of generality that $L > \|\rho_0\|_{L^\infty(\Omega)}$, the (upper) cut-off parameter L can be eliminated from (1.43) by recalling that $\beta^L(r) := \min\{r, L\}$ and noting that $\beta^L(r) = r$ for $L > r$.

Hence, by assuming without loss of generality that $L > \|\rho_0\|_{L^\infty(\Omega)}$, the semidiscrete-in-time formulation of our problem becomes the following:

$$\begin{aligned} & \text{Find } \rho^{\Delta t}(\cdot, t) \in V = H^1(\Omega), \, t \in (0, T], \text{ such that} \\ & \int_0^T \int_{\Omega} \frac{\partial \rho^{\Delta t}}{\partial t} \phi \, dx \, dt = - \int_0^T \int_{\Omega} \nabla \rho^{\Delta t, +} \cdot \nabla \phi \, dx \, dt + \int_0^T \int_{\Omega} \rho^{\Delta t, +} \nabla c^{\Delta t, +} \cdot \nabla \phi \, dx \, dt \quad (1.51a) \\ & \text{for all } \phi \in L^1(0, T; V), \end{aligned}$$

subject to the initial condition $\rho^{\Delta t}(x, 0) = \rho^0(x)$ for a.e. $x \in \Omega$, where $c^{\Delta t, +}(\cdot, t) \in H_*^1(\Omega)$ for all $t \in (0, T]$ and satisfies

$$-(-\Delta_N)^s c^{\Delta t, +}(\cdot, t) = (\rho^{\Delta t, +})^*(\cdot, t) \quad \text{in } \Omega \quad (1.51b)$$

for all $t \in (0, T]$, and the definitions of $\rho^{\Delta t, (\pm)}$ are analogous to those of $\rho_L^{\Delta t, (\pm)}$ stated in (1.40).

We can now start to derive a bound that is uniform in Δt . Our candidate test function will be $\phi = \chi_{[0, t]} G'(\rho^{\Delta t, +})$, where $\chi_{[0, t]}$ denotes the characteristic function of the interval $[0, t]$. However, since $\lim_{r \rightarrow 0+} G'(r) = +\infty$, we need to be careful because, although the convergence results (1.37) ensure that $\rho^{\Delta t, +}$ is nonnegative a.e. on $\Omega \times (0, T]$, there is no reason why $\rho^{\Delta t, +}$ should be strictly positive a.e. on $\Omega \times (0, T]$. We shall circumvent this problem by choosing as a test function $\chi_{[0, t]} G'(\rho^{\Delta t, +} + \alpha)$ where $\alpha > 0$. In this way $G'(\rho^{\Delta t, +} + \alpha)$ and $G''(\rho^{\Delta t, +} + \alpha)$ will be well defined. After a series of manipulations we shall arrive at a bound involving $G(\rho^{\Delta t, +} + \alpha)$ only. At that point we will be able to pass to the limit as $\alpha \rightarrow 0+$, noting that, unlike $G'(\rho^{\Delta t, +})$ and $G''(\rho^{\Delta t, +})$, which are only defined when $\rho^{\Delta t, +}$ is positive, the function $G(\rho^{\Delta t, +})$ is well defined for nonnegative $\rho^{\Delta t, +}$.

Thus we take $\alpha \in (0, 1)$ and we choose $\phi = \chi_{[0, t]} G'(\rho^{\Delta t, +} + \alpha)$, with $t = t_n$, $n \in \{1, \dots, N\}$. We have

$$\begin{aligned} & \underbrace{\int_0^T \int_{\Omega} \frac{\partial \rho^{\Delta t}}{\partial t} \chi_{[0, t_n]} G'(\rho^{\Delta t, +} + \alpha) \, dx \, dt}_{\textcircled{1}} + \underbrace{\int_0^T \int_{\Omega} \nabla \rho^{\Delta t, +} \cdot \nabla \chi_{[0, t_n]} G'(\rho^{\Delta t, +} + \alpha) \, dx \, dt}_{\textcircled{2}} \\ & = \underbrace{\int_0^T \int_{\Omega} \rho^{\Delta t, +} \nabla c^{\Delta t, +} \cdot \nabla \chi_{[0, t_n]} G'(\rho^{\Delta t, +} + \alpha) \, dx \, dt}_{\textcircled{3}}. \end{aligned}$$

Let us now manipulate the three terms one at a time. First, by Taylor expansion with a remainder of the function

$$r \in [0, \infty) \mapsto G(r + \alpha) \in [0, \infty),$$

we have that, for any $b \in [0, \infty)$,

$$(r - b)G'(r + \alpha) = G(r + \alpha) - G(b + \alpha) + \frac{1}{2}(r - b)^2 G''(\theta r + (1 - \theta)b + \alpha),$$

with $\theta \in (0, 1)$. Noting that for $t \in [0, T]$ the function $t \mapsto \rho^{\Delta t}(\cdot, t)$ is, by definition, piecewise affine relative to the partition $0 = t_0 < t_1 < \dots < t_N = T$ of the interval $[0, T]$, it follows that

$$\begin{aligned} \textcircled{1} &= \int_{\Omega} G(\rho^{\Delta t, +}(x, t_n) + \alpha) \, dx - \int_{\Omega} G(\rho^0(x) + \alpha) \, dx \\ &+ \frac{1}{2\Delta t} \int_0^{t_n} \int_{\Omega} G''(\theta \rho^{\Delta t, +} + (1 - \theta)\rho^{\Delta t, -} + \alpha)(\rho^{\Delta t, +} - \rho^{\Delta t, -})^2 \, dx \, d\tau. \end{aligned}$$

As $G''(r + \alpha) = \frac{1}{r + \alpha}$ for all $r \geq 0$ and (1.50) implies that $G''(\theta \rho^{\Delta t, +} + (1 - \theta)\rho^{\Delta t, -} + \alpha) \geq \frac{1}{\|\rho_0\|_{L^\infty(\Omega)} + \alpha}$ almost everywhere in $\Omega \times (0, T)$ it follows that

$$\begin{aligned} \textcircled{1} &\geq \int_{\Omega} G(\rho^{\Delta t, +}(x, t_n) + \alpha) \, dx - \int_{\Omega} G(\rho^0(x) + \alpha) \, dx \\ &+ \frac{1}{2\Delta t (\|\rho_0\|_{L^\infty(\Omega)} + \alpha)} \int_0^{t_n} \int_{\Omega} (\rho^{\Delta t, +} - \rho^{\Delta t, -})^2 \, dx \, d\tau. \end{aligned}$$

For the second term we have

$$\textcircled{2} = \int_0^{t_n} \int_{\Omega} G''(\rho^{\Delta t,+} + \alpha) |\nabla \rho^{\Delta t,+}|^2 dx d\tau = \int_0^{t_n} \int_{\Omega} \frac{|\nabla \rho^{\Delta t,+}|^2}{\rho^{\Delta t,+} + \alpha} dx d\tau,$$

again, since $(G^L)''(r + \alpha) = \frac{1}{r + \alpha}$ for all $r \geq 0$.

For the third term we have

$$\textcircled{3} = \int_0^{t_n} \int_{\Omega} \frac{\rho^{\Delta t,+}}{\rho^{\Delta t,+} + \alpha} \nabla c^{\Delta t,+} \cdot \nabla \rho^{\Delta t,+} dx d\tau.$$

Putting everything together we therefore have that

$$\begin{aligned} & \int_{\Omega} G(\rho^{\Delta t,+}(x, t_n) + \alpha) dx + \frac{1}{2\Delta t (\|\rho_0\|_{L^\infty(\Omega)} + \alpha)} \int_0^{t_n} \int_{\Omega} (\rho^{\Delta t,+} - \rho^{\Delta t,-})^2 dx d\tau \\ & \quad + \int_0^{t_n} \int_{\Omega} \frac{|\nabla \rho^{\Delta t,+}|^2}{\rho^{\Delta t,+} + \alpha} dx d\tau \\ & \quad - \int_0^{t_n} \int_{\Omega} \frac{\rho^{\Delta t,+}}{\rho^{\Delta t,+} + \alpha} \nabla c^{\Delta t,+} \cdot \nabla \rho^{\Delta t,+} dx d\tau \\ & \leq \int_{\Omega} G(\rho^0(x) + \alpha) dx. \end{aligned} \tag{1.52}$$

We can now pass to the limit as $\alpha \rightarrow 0_+$ to obtain the following bound for $n = 1, \dots, N$, which is uniform in Δt thanks to (1.29):

$$\begin{aligned} & \int_{\Omega} G(\rho^{\Delta t,+}(x, t_n)) dx + \frac{1}{2\Delta t \|\rho_0\|_{L^\infty(\Omega)}} \int_0^{t_n} \int_{\Omega} (\rho^{\Delta t,+} - \rho^{\Delta t,-})^2 dx d\tau \\ & \quad + 4 \int_0^{t_n} \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t,+}} \right|^2 dx d\tau - \int_0^{t_n} \int_{\Omega} \nabla c^{\Delta t,+} \cdot \nabla \rho^{\Delta t,+} dx d\tau \\ & \leq \int_{\Omega} G(\rho^0(x)) dx \leq \int_{\Omega} G(\rho_0) dx =: C(\rho_0). \end{aligned} \tag{1.53}$$

Finally we notice that, for $t \in (0, T]$,

$$\int_{\Omega} \nabla c^{\Delta t,+}(x, t) \cdot \nabla \rho^{\Delta t,+}(x, t) dx \leq 0; \tag{1.54}$$

this can be proved by using the density of $C^\infty(\overline{\Omega})$ functions in $H^1(\Omega)$ and a similar argument as the one contained in the proof of Lemma 1.16 to show the nonpositivity of the term (1.46).

We therefore have, for $n = 1, \dots, N$, that

$$\begin{aligned} & \int_{\Omega} G(\rho^{\Delta t,+}(x, t_n)) dx + \frac{1}{2\Delta t \|\rho_0\|_{L^\infty(\Omega)}} \int_0^{t_n} \int_{\Omega} (\rho^{\Delta t,+} - \rho^{\Delta t,-})^2 dx d\tau \\ & \quad + 4 \int_0^{t_n} \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t,+}} \right|^2 dx d\tau \leq C(\rho_0). \end{aligned} \tag{1.55}$$

Using property (1.29) we can supplement the above inequality with additional bounds. The first of these is arrived at by noticing that

$$\begin{aligned}
4 \int_0^T \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t, -}} \right|^2 dx dt &= 4\Delta t \int_{\Omega} \left| \nabla \sqrt{\rho^0} \right|^2 dx + 4 \int_{\Delta t}^T \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t, -}} \right|^2 dx dt \\
&= 4\Delta t \int_{\Omega} \left| \nabla \sqrt{\rho^0} \right|^2 dx + 4 \int_0^{T-\Delta t} \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t, +}} \right|^2 dx dt \\
&\leq \int_{\Omega} G(\rho_0) dx + 4 \int_0^{T-\Delta t} \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t, +}} \right|^2 dx dt \leq C_{\star},
\end{aligned}$$

where in the two inequalities appearing in the last line we used (1.29) and (1.55), respectively; here and henceforth $C_{\star}$ signifies a generic positive constant, independent of Δt .

A simple calculation then shows that we can also get a similar inequality for $\rho^{\Delta t}$, and therefore we have the uniform bound

$$4 \int_0^T \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t, (\pm)}} \right|^2 dx dt \leq C_{\star}. \quad (1.56)$$

At this stage we can also obtain a uniform bound on the norm of $c^{\Delta t, +}$. By choosing $-\chi_{[0, t_n]} c^{\Delta t, +}$ as a test function in (1.51a) and recalling (1.42) we have, for each $n \in \{1, \dots, N\}$, that

$$\begin{aligned}
& - \int_0^{t_n} \int_{\Omega} \frac{\partial(\rho^{\Delta t})^*}{\partial t} c^{\Delta t, +} dx d\tau \\
& + \int_0^{t_n} \int_{\Omega} \rho^{\Delta t, +} \nabla c^{\Delta t, +} \cdot \nabla c^{\Delta t, +} dx d\tau = \int_0^{t_n} \int_{\Omega} \nabla \rho^{\Delta t, +} \cdot \nabla c^{\Delta t, +} dx d\tau,
\end{aligned}$$

which is equivalent to

$$\begin{aligned}
& \underbrace{- \int_0^{t_n} \int_{\Omega} \frac{\partial(\rho^{\Delta t})^*}{\partial t} c^{\Delta t} dx d\tau}_{\textcircled{1}} + \underbrace{\int_0^{t_n} \int_{\Omega} \frac{\partial(\rho^{\Delta t})^*}{\partial t} (c^{\Delta t} - c^{\Delta t, +}) dx d\tau}_{\textcircled{2}} \\
& + \int_0^{t_n} \int_{\Omega} \rho^{\Delta t, +} \left| \nabla c^{\Delta t, +} \right|^2 dx d\tau = \int_0^{t_n} \int_{\Omega} \nabla \rho^{\Delta t, +} \cdot \nabla c^{\Delta t, +} dx d\tau.
\end{aligned}$$

The idea at this point is to extract from term $\textcircled{1}$ the $\mathbb{H}^s$ norm of $c^{\Delta t, +}$ in a similar way as we did in (1.17). Expanding and using (1.41) and (1.42), thanks to the fact that the fractional

Laplacian is an operator acting only in space, we have for each $n \in \{1, \dots, N\}$ that

$$\begin{aligned}
\textcircled{1} &= - \sum_{m=1}^n \int_{t_{m-1}}^{t_m} \frac{\partial(\rho^{\Delta t})^*}{\partial t} c^{\Delta t} dx d\tau = - \sum_{m=1}^n \int_{t_{m-1}}^{t_m} \int_{\Omega} \frac{(\rho^{\Delta t,+})^* - (\rho^{\Delta t,-})^*}{\Delta t} c^{\Delta t} dx d\tau \\
&= \sum_{m=1}^n \int_{\Omega} \frac{(\rho^m)^* - (\rho^{m-1})^*}{\Delta t} \left(\int_{t_{m-1}}^{t_m} \frac{t - t_{m-1}}{\Delta t} (-\Delta_N)^{-s} (\rho^m)^* d\tau \right. \\
&\quad \left. + \int_{t_{m-1}}^{t_m} \frac{t_m - t}{\Delta t} (-\Delta_N)^{-s} (\rho^{m-1})^* d\tau \right) dx \\
&= \frac{1}{2} \sum_{m=1}^n \int_{\Omega} ((\rho^m)^* - (\rho^{m-1})^*) ((-\Delta_N)^{-s} (\rho^m)^* + (-\Delta_N)^{-s} (\rho^{m-1})^*) dx \\
&= \frac{1}{2} \int_{\Omega} (\rho^n)^* (-\Delta_N)^{-s} (\rho^n)^* dx - \frac{1}{2} \int_{\Omega} (\rho^0)^* (-\Delta_N)^{-s} (\rho^0)^* dx \\
&= -\frac{1}{2} \int_{\Omega} (\rho^{\Delta t,+})^*(x, t_n) c^{\Delta t,+}(x, t_n) dx + \frac{1}{2} \int_{\Omega} (\rho^0)^*(x) c^0(x) dx \\
&= \frac{1}{2} \int_{\Omega} (-\Delta_N)^s c^{\Delta t,+}(x, t_n) c^{\Delta t,+}(x, t_n) dx - \frac{1}{2} \int_{\Omega} (-\Delta_N)^s c^0(x) c^0(x) dx.
\end{aligned}$$

We now wish to show that the term $\textcircled{2}$ is nonnegative. We first notice that on the interval $[t_{n-1}, t_n]$, by proceeding similarly as in the case of term $\textcircled{1}$, we have by linearity that

$$c^{\Delta t} - c^{\Delta t,+} = \frac{t - t_n}{\Delta t} (c^{\Delta t,+} - c^{\Delta t,-}) = \frac{t_n - t}{\Delta t} (-\Delta_N)^{-s} ((\rho^{\Delta t,+})^* - (\rho^{\Delta t,-})^*).$$

Therefore, we have that

$$\begin{aligned}
\textcircled{2} &= \int_0^{t_n} \int_{\Omega} \frac{(\rho^{\Delta t,+})^* - (\rho^{\Delta t,-})^*}{\Delta t} (c^{\Delta t} - c^{\Delta t,+}) dx d\tau \\
&= \sum_{m=1}^n \int_{t_{m-1}}^{t_m} \int_{\Omega} \frac{(\rho^{\Delta t,+})^* - (\rho^{\Delta t,-})^*}{\Delta t} \frac{t_m - t}{\Delta t} (-\Delta_N)^{-s} ((\rho^{\Delta t,+})^* - (\rho^{\Delta t,-})^*) dx d\tau \\
&= \sum_{m=1}^n \int_{t_{m-1}}^{t_m} \frac{t_m - t}{\Delta t^2} \int_{\Omega} ((\rho^{\Delta t,+})^* - (\rho^{\Delta t,-})^*) (-\Delta_N)^{-s} ((\rho^{\Delta t,+})^* - (\rho^{\Delta t,-})^*) dx d\tau.
\end{aligned}$$

Since the inverse fractional Laplacian is a positive operator, we have that $\textcircled{2} \geq 0$, and therefore

$$\begin{aligned}
&\frac{1}{2} \int_{\Omega} (-\Delta_N)^s c^{\Delta t,+}(x, t_n) c^{\Delta t,+}(x, t_n) dx + \int_0^{t_n} \int_{\Omega} \rho^{\Delta t,+} |\nabla c^{\Delta t,+}|^2 dx d\tau \\
&\quad - \int_0^{t_n} \int_{\Omega} \nabla \rho^{\Delta t,+} \cdot \nabla c^{\Delta t,+} dx d\tau \leq \frac{1}{2} \int_{\Omega} (-\Delta_N)^s c^0(x) c^0(x) dx,
\end{aligned} \tag{1.57}$$

which means, by (1.54), that

$$\begin{aligned}
&\frac{1}{2} \int_{\Omega} (-\Delta_N)^s c^{\Delta t,+}(x, t_n) c^{\Delta t,+}(x, t_n) dx + \int_0^{t_n} \int_{\Omega} \rho^{\Delta t,+} |\nabla c^{\Delta t,+}|^2 dx d\tau \\
&\leq \frac{1}{2} \int_{\Omega} (-\Delta_N)^s c^0(x) c^0(x) dx
\end{aligned}$$

for all $n = 1, \dots, N$. Notice that, by (A.3),

$$\int_{\Omega} (-\Delta_N)^s c^0 c^0 dx = \|c^0\|_{\mathbb{H}^s(\Omega)}^2 \leq C \|\rho^0\|_{L^2(\Omega)}^2 \leq C \|\rho_0\|_{L^2(\Omega)}^2 = C_{\star}.$$

Therefore we have the following overall (uniform in Δt) bound on $c^{\Delta t,+}$:

$$\sup_{t \in [0, T]} \int_{\Omega} (-\Delta_N)^s c^{\Delta t,+}(t) c^{\Delta t,+}(t) dx + \int_0^t \int_{\Omega} \rho^{\Delta t,+} |\nabla c^{\Delta t,+}|^2 dx dt \leq C_{\star}. \quad (1.58)$$

We observe that (1.53) in conjunction with (1.57) leads, for any $n \in \{1, \dots, N\}$, to the following bound on the energy functional that we defined in (1.10):

$$\begin{aligned} E(\rho^{\Delta t,+}(t_n)) - E(\rho^0) &= \int_{\Omega} G(\rho^{\Delta t,+}(x, t_n)) dx - \frac{1}{2} \int_{\Omega} (\rho^{\Delta t,+})^*(x, t_n) c^{\Delta t,+}(x, t_n) dx \\ &\quad - \int_{\Omega} G(\rho^0(x)) dx + \frac{1}{2} \int_{\Omega} (\rho^0)^*(x) c^0(x) dx \\ &\leq -4 \int_0^{t_n} \int_{\Omega} |\nabla \sqrt{\rho^{\Delta t,+}}|^2 dx dt + 2 \int_0^{t_n} \int_{\Omega} \nabla \rho^{\Delta t,+} \cdot \nabla c^{\Delta t,+} dx dt \\ &\quad - \int_0^{t_n} \int_{\Omega} \rho^{\Delta t,+} |\nabla c^{\Delta t,+}|^2 dx dt. \end{aligned} \quad (1.59)$$

The inequality (1.59) can be rewritten, for any $n \in \{1, \dots, N\}$, as

$$E(\rho^{\Delta t,+}(t_n)) + \int_0^{t_n} \int_{\Omega} |2\nabla \sqrt{\rho^{\Delta t,+}} - \sqrt{\rho^{\Delta t,+}} \nabla c^{\Delta t,+}|^2 dx dt \leq E(\rho^0). \quad (1.60)$$

Because $|2\nabla \sqrt{\rho^{\Delta t,+}} - \sqrt{\rho^{\Delta t,+}} \nabla c^{\Delta t,+}|^2 = \rho^{\Delta t,+} |\nabla(\log \rho^{\Delta t,+} - c^{\Delta t,+})|^2$, the inequality (1.60) can be seen as a temporally semi-discrete counterpart of the time-integral in the (formal) free energy identity (1.11).

We shall assume throughout the rest of the section that the test functions belong to the function space $L^2(0, T, W^{1,\infty}(\Omega))$. Our objective is to derive a (uniform in Δt) bound on the time-derivative of $\rho^{\Delta t}$ in terms of the $L^2(0, T, W^{1,\infty}(\Omega))$ norm of the test function, followed by the use of Sobolev embedding, which will enable us to apply a variant of the Aubin–Lions compactness lemma, known as Dubinskii’s compactness theorem. From (1.51a) we have that, for a test function $\phi \in L^2(0, T, W^{1,\infty}(\Omega))$,

$$\left| \int_0^T \int_{\Omega} \frac{\partial \rho^{\Delta t}}{\partial t} \phi dx dt \right| \leq \underbrace{\left| \int_0^T \int_{\Omega} \nabla \rho^{\Delta t,+} \cdot \nabla \phi dx dt \right|}_{\textcircled{1}} + \underbrace{\left| \int_0^T \int_{\Omega} \rho^{\Delta t,+} \nabla c^{\Delta t,+} \cdot \nabla \phi dx dt \right|}_{\textcircled{2}}.$$

We recall that we have

$$\rho^{\Delta t,(\pm)} \geq 0 \quad \text{a.e. on } \Omega \times (0, T), \quad \text{and} \quad (1.61a)$$

$$\frac{1}{|\Omega|} \int_{\Omega} \rho^{\Delta t,(\pm)}(t) = 1 \quad \text{for a.e. } t \in (0, T). \quad (1.61b)$$

Moreover we notice that the bound on the first term on the left-hand side of (1.55) gives us a (uniform in Δt) bound on the $L^\infty(0, T; L^1(\Omega))$ norm of $\rho^{\Delta t,+}$, because the function $r \in [0, \infty) \mapsto G(r) \in [0, \infty)$ has superlinear growth as $r \rightarrow +\infty$.

For the term ① we then have by (1.55) and (1.61) that

$$\begin{aligned}
① &\leq \int_0^T \|\nabla \phi\|_{L^\infty(\Omega)} \int_\Omega |\nabla \rho^{\Delta t,+}| \, dx \, dt = 2 \int_0^T \|\nabla \phi\|_{L^\infty(\Omega)} \int_\Omega \sqrt{\rho^{\Delta t,+}} \left| \nabla \sqrt{\rho^{\Delta t,+}} \right| \, dx \, dt \\
&\leq 2 \int_0^T \|\nabla \phi\|_{L^\infty(\Omega)} \left(\int_\Omega \rho^{\Delta t,+} \, dx \right)^{\frac{1}{2}} \left(\int_\Omega \left| \nabla \sqrt{\rho^{\Delta t,+}} \right|^2 \, dx \right)^{\frac{1}{2}} \, dt \\
&\leq C_\star \left(\int_0^T \|\nabla \phi\|_{L^\infty(\Omega)}^2 \, dt \right)^{\frac{1}{2}}.
\end{aligned}$$

For the term ② we recall the bound on the second term on the left-hand side of (1.58) together with (1.55); with a similar computation as for term ① above we get

$$② \leq C_\star \left(\int_0^T \|\nabla \phi\|_{L^\infty(\Omega)}^2 \, dt \right)^{\frac{1}{2}}.$$

By combining the bounds on the terms ① and ② and noting that by the Sobolev embedding theorem $H^{d+1}(\Omega)$ is continuously embedded in $W^{1,\infty}(\Omega)$ for $d = 2, 3$, we then have that

$$\left| \int_0^T \int_\Omega \frac{\partial \rho^{\Delta t}}{\partial t} \phi \, dx \, dt \right| \leq C_\star \left(\int_0^T \|\nabla \phi\|_{L^\infty(\Omega)}^2 \, dt \right)^{\frac{1}{2}} \leq C_\star \left(\int_0^T \|\phi\|_{H^{d+1}(\Omega)}^2 \, dt \right)^{\frac{1}{2}}. \quad (1.62)$$

We are now ready to take the limit as $\Delta t \rightarrow 0_+$. Our main tool to this end will be Dubinskiĭ's compactness theorem in seminormed sets, which we shall state in the next subsection; cf. [94] and [24].

1.3.1 Dubinskiĭ's compactness theorem

Let $\mathcal{A}$ be a linear space over the field $\mathbb{R}$ of real numbers, which will be referred as *ambient space*, and suppose that $\mathcal{C}$ is a subset of $\mathcal{A}$ such that,

$$\text{for all } \varphi \in \mathcal{C} \text{ and } c \in \mathbb{R}_{\geq 0}, \quad c\varphi \in \mathcal{C}. \quad (1.63)$$

Suppose further that each element φ of a set $\mathcal{C}$ with property (1.63) is assigned a certain real number, denoted by $[\varphi]_{\mathcal{C}}$, such that

1. $[\varphi]_{\mathcal{C}} \geq 0$, and $[\varphi]_{\mathcal{C}} = 0$ if, and only if, $\varphi = 0$;
2. $[c\varphi]_{\mathcal{C}} = c[\varphi]_{\mathcal{C}}$ for all $c \in \mathbb{R}_{\geq 0}$.

A subset $\mathcal{C}$ satisfying (1.63), equipped with $[\cdot]_{\mathcal{C}}$ satisfying these two properties is referred to as a *seminormed set*. The set $\mathcal{C}$ can be visualised as a cone, as illustrated in Figure 1.3.

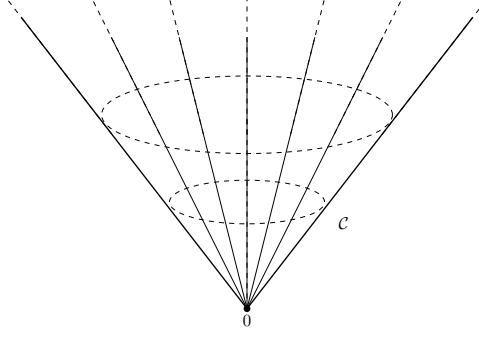


Figure 1.3: Seminormed set.

Theorem 1.18 (c.f. [24]). *Suppose that $\mathcal{A}_0$ and $\mathcal{A}_1$ are Banach spaces, $\mathcal{A}_0 \hookrightarrow \mathcal{A}_1$ (i.e., $\mathcal{A}_0$ is continuously embedded in $\mathcal{A}_1$), and $\mathcal{C}$ is a seminormed set contained in $\mathcal{A}_0$ such that $\mathcal{C}$ is compactly embedded in $\mathcal{A}_0$. Consider the set*

$$\mathcal{Y} := \left\{ \varphi : [0, T] \rightarrow \mathcal{C} : [\varphi]_{L^p(0, T; \mathcal{C})} + \left\| \frac{d\varphi}{dt} \right\|_{L^{p_1}(0, T; \mathcal{A}_1)} < \infty \right\},$$

where $1 \leq p \leq \infty$, $1 \leq p_1 \leq \infty$, $\|\cdot\|_{\mathcal{A}_1}$ is the norm of $\mathcal{A}_1$ and $\frac{d\varphi}{dt}$ is understood in the sense of $\mathcal{A}_1$ -valued distributions on the open interval $(0, T)$. Then $\mathcal{Y}$, with

$$[\varphi]_{\mathcal{Y}} := [\varphi]_{L^p(0, T; \mathcal{C})} + \left\| \frac{d\varphi}{dt} \right\|_{L^{p_1}(0, T; \mathcal{A}_1)},$$

is a seminormed set in $L^p(0, T; \mathcal{A}_0) \cap W^{1, p_1}(0, T; \mathcal{A}_1)$, and $\mathcal{Y}$ is compactly embedded in $L^p(0, T; \mathcal{A}_0)$ if either $1 \leq p \leq \infty$ and $1 < p_1 < \infty$, or if $1 \leq p < \infty$ and $p_1 = 1$.

In our current setting we shall apply Dubinskii's theorem, as in [21], by selecting

$$\mathcal{A}_0 = L^1(\Omega), \text{ with the usual Lebesgue norm } \|\varphi\|_{\mathcal{A}_0} := \int_{\Omega} |\varphi| \, dx$$

and

$$\mathcal{C} = \left\{ \phi \in \mathcal{A}_0 : \phi \geq 0 \text{ with } \int_{\Omega} |\nabla \sqrt{\phi}|^2 \, dx < \infty \right\};$$

and, for $\varphi \in \mathcal{C}$, we define

$$[\varphi]_{\mathcal{C}} := \|\varphi\|_{\mathcal{A}_0} + \int_{\Omega} |\nabla \sqrt{\varphi}|^2 \, dx.$$

It is a straightforward matter to confirm that (1.63) and properties 1. and 2. stated above hold, rendering $\mathcal{C}$ a seminormed subset of the ambient space $\mathcal{A}_0 = L^1(\Omega)$. Finally we put

$$\mathcal{A}_1 = H^{-\beta}(\Omega) := [H^{\beta}(\Omega)]' \quad \text{with } \beta = d + 1,$$

equipped with the dual norm $\|\varphi\|_{\mathcal{A}_1} := \|\varphi\|_{H^{-\beta}(\Omega)}$. The choice of $\mathcal{A}_1$ is motivated by the (continuous) Sobolev embedding

$$H^{\beta}(\Omega) \hookrightarrow W^{1, \infty}(\Omega).$$

In this way the right-hand side of (1.62) can be further bounded by a constant multiple of $\|\phi\|_{L^2(0,T;H^\beta(\Omega))}$. The Banach spaces $\mathcal{A}_0$ and $\mathcal{A}_1$ and the seminormed set $\mathcal{C}$ then satisfy the conditions of Theorem 1.18, with $\mathcal{C} \hookrightarrow \mathcal{A}_0$ compactly and $\mathcal{A}_0 \hookrightarrow \mathcal{A}_1$ (cf. [21]).²

We shall also make use of the next lemma, whose proof via Hölder's inequality is straightforward and is therefore omitted.

Lemma 1.19. *Suppose that a sequence $\{\varphi_n\}_{n \geq 1}$ converges strongly in $L^1(0,T;L^1(\Omega))$ to a function $\varphi \in L^1(0,T;L^1(\Omega))$, and is bounded in $L^\infty(0,T;L^\infty(\Omega))$; namely, there exists a $K > 0$ such that $\|\varphi_n\|_{L^\infty(0,T;L^\infty(\Omega))} \leq K$ for all $n \geq 1$. Then $\varphi \in L^p(0,T;L^q(\Omega))$ for all $p, q \in [1, \infty)$ and the sequence $\{\varphi_n\}_{n \geq 1}$ converges to φ strongly in $L^p(0,T;L^q(\Omega))$ for all $p, q \in [1, \infty)$.*

1.3.2 Passage to the limit $\Delta t \rightarrow 0_+$

We begin by collecting the Δt -independent bounds (1.55), (1.56), (1.62); we have shown that there exists a constant C_* , independent of Δt , such that

$$\begin{aligned} \sup_{t \in (0,T]} \int_{\Omega} G(\rho^{\Delta t,+}(t)) \, dx + \frac{1}{\Delta t} \int_0^T \int_{\Omega} (\rho^{\Delta t,+} - \rho^{\Delta t,-})^2 \, dx \, dt \\ + \int_0^T \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t,(\pm)}} \right|^2 \, dx \, dt + \int_0^T \left\| \frac{\partial \rho^{\Delta t}}{\partial t} \right\|_{H^{-\beta}(\Omega)}^2 \, dt \leq C_*. \end{aligned} \quad (1.64)$$

In the proof of the next theorem we shall require a technical result concerning weakly continuous and weak-* continuous functions. Suppose to this end that X is a Banach space and let X' be the (continuous) dual space of X . Let us denote by $C_w([0,T];X)$ the set of all weakly continuous functions that map $[0,T]$ into X , namely the set of all functions $\eta \in L^\infty(0,T;X)$ such that $t \in [0,T] \mapsto \langle \varphi, \eta(t) \rangle_X \in \mathbb{R}$ is continuous on $[0,T]$ for all $\varphi \in X'$. Whenever X has a predual E , we shall denote by $C_{w^*}([0,T];X)$ the set of all functions $\eta \in L^\infty(0,T;X)$ such that $t \in [0,T] \mapsto \langle \eta(t), \zeta \rangle \in \mathbb{R}$ is continuous on $[0,T]$ for all $\zeta \in E$. We will use [25, Lemma 2.1], that we cite here.

Lemma 1.20. *Suppose that X and E are Banach spaces.*

- (a) *Assume that the space X is reflexive and is continuously embedded in a Banach space Y ; then $L^\infty(0,T;X) \cap C_w([0,T];Y) = C_w([0,T];X)$.*
- (b) *Assume that X has a separable predual E and the Banach space Y has a predual F such that F is continuously embedded in E ; then, $L^\infty(0,T;X) \cap C_{w^*}([0,T];Y) = C_{w^*}([0,T];X)$.*

We are now ready to pass to the limit $\Delta t \rightarrow 0_+$.

²The continuous embedding of $\mathcal{A}_0$ into $\mathcal{A}_1$ follows from the following abstract result, whose proof is straightforward. Let X and Y be normed linear spaces with (continuous) dual spaces X' and Y' , respectively, and let $i : X \rightarrow Y'$ be a continuous embedding. Then the mapping $j : Y \rightarrow X'$, defined by $\langle j(y), x \rangle := \langle y, i(x) \rangle$, is continuous. Moreover, if $i(X)$ is weak-* dense in Y' , then j is injective, i.e., j is a continuous embedding. We take $X = H^\beta(\Omega)$ with $\beta = d+1$, $Y = \mathcal{A}_0 = L^1(\Omega)$, and note that $Y' = L^\infty(\Omega)$.

Theorem 1.21. *There exists a subsequence of $\{\rho^{\Delta t(\pm)}\}_{\Delta t > 0}$ (not indicated) and a function $\widehat{\rho}$ such that*

$$\widehat{\rho} \in L^\infty(0, T; L^\infty(\Omega)) \cap H^1(0, T; H^{-\beta}(\Omega)), \quad \beta = d + 1,$$

with $\widehat{\rho} \geq 0$ almost everywhere on $\Omega \times (0, T)$ and $\frac{1}{|\Omega|} \int_\Omega \widehat{\rho}(x, t) dx = 1$ for a.e. $t \in [0, T]$, and $\widehat{c}(\cdot, t) \in \mathbb{H}^s(\Omega) \cap H_^1(\Omega)$ defined as $-(-\Delta_N)^s \widehat{c}(\cdot, t) = \widehat{\rho}^*(\cdot, t)$ in Ω for $t \in (0, T]$ such that, for all $p \in [1, \infty)$,*

$$\rho^{\Delta t(\pm)} \rightarrow \widehat{\rho} \quad \text{strongly in } L^p(0, T; L^1(\Omega)), \quad (1.65a)$$

$$\nabla \sqrt{\rho^{\Delta t(\pm)}} \rightarrow \nabla \sqrt{\widehat{\rho}} \quad \text{weakly in } L^2(0, T; L^2(\Omega; \mathbb{R}^d)), \quad (1.65b)$$

$$\frac{\partial \rho^{\Delta t}}{\partial t} \rightarrow \frac{\partial \widehat{\rho}}{\partial t} \quad \text{weakly in } L^2(0, T; H^{-\beta}(\Omega)), \quad (1.65c)$$

$$\rho^{\Delta t(\pm)} \rightarrow \widehat{\rho} \quad \text{weakly-* in } L^\infty(0, T; L^\infty(\Omega)), \quad (1.65d)$$

$$\rho^{\Delta t(\pm)} \rightarrow \widehat{\rho} \quad \text{strongly in } L^p(0, T; L^p(\Omega)), \quad (1.65e)$$

$$c^{\Delta t(\pm)} \rightarrow \widehat{c} \quad \text{strongly in } L^p(0, T; \mathbb{H}^s(\Omega)), \quad (1.65f)$$

$$\nabla c^{\Delta t, +} \rightarrow \nabla \widehat{c} \quad \text{weakly in } L^2(0, T; L^2(\Omega; \mathbb{R}^d)). \quad (1.65g)$$

The function $\widehat{\rho}$ is a global weak solution to the problem

$$-\int_0^T \int_\Omega \widehat{\rho} \frac{\partial \phi}{\partial t} dx dt + \int_0^T \int_\Omega \nabla \widehat{\rho} \cdot \nabla \phi dx dt - \int_0^T \int_\Omega \widehat{\rho} \nabla \widehat{c} \cdot \nabla \phi dx dt = \int_\Omega \rho_0 \phi|_{t=0} dx \quad (1.65h)$$

for all $\phi \in W^{1,1}(0, T; H^\beta(\Omega))$ such that $\phi(\cdot, T) = 0$.

In addition, the function $\widehat{\rho}$ is weak- continuous as a mapping from $[0, T]$ to $L^\infty(\Omega)$ and it is weakly continuous as a mapping from $[0, T]$ to $L^1(\Omega)$. The energy functional $E(\cdot)$ defined in (1.10) satisfies the inequality*

$$E(\widehat{\rho}(t)) + \int_0^t \int_\Omega \left| 2\nabla \sqrt{\widehat{\rho}} - \sqrt{\widehat{\rho}} \nabla \widehat{c} \right|^2 dx d\tau \leq E(\rho_0), \quad (1.65i)$$

for a.e. $t \in [0, T]$.

Proof. We choose $\mathcal{A}_0, \mathcal{A}_1$ and $\mathcal{C}$ as in the discussion following the statement of Dubinskiĭ's theorem (Theorem 1.18). Then, by taking $p = 1$ and $p_1 = 2$ we have that

$$\left\{ \varphi : [0, T] \rightarrow \mathcal{C} : [\varphi]_{L^p(0, T; \mathcal{C})} + \left\| \frac{d\varphi}{dt} \right\|_{L^{p_1}(0, T; \mathcal{A}_1)} < \infty \right\}$$

is compactly embedded in $L^1(0, T; \mathcal{A}_0) = L^1(0, T; L^1(\Omega))$. By using the bounds on the last two terms on the left-hand side of (1.64), we have that there exists a subsequence of $\{\rho^{\Delta t}\}_{\Delta t > 0}$ (not indicated), which converges strongly in $L^1(0, T; L^1(\Omega))$ to an element $\widehat{\rho} \in L^1(0, T; L^1(\Omega))$ as $\Delta t \rightarrow 0$. The strong convergence in $L^1(0, T; L^1(\Omega))$ ensures almost everywhere convergence of a

subsequence (not indicated) to $\widehat{\rho}$. We have by (1.40) and the bound on the second term on the left-hand side of (1.64) that

$$\left(\int_0^T \int_{\Omega} |\rho^{\Delta t} - \rho^{\Delta t,+}| \, dx \, dt \right)^2 \leq T|\Omega| \int_0^T \int_{\Omega} (\rho^{\Delta t,+} - \rho^{\Delta t,-})^2 \, dx \, dt \leq C_{\star} T |\Omega| \Delta t. \quad (1.66)$$

We apply the triangle inequality in $L^1(0, T; L^1(\Omega))$, together with the strong convergence of the sequence $\{\rho^{\Delta t}\}_{\Delta t > 0}$ in $L^1(0, T; L^1(\Omega))$ to deduce strong convergence in $L^1(0, T; L^1(\Omega))$ to the same element $\widehat{\rho} \in L^1(0, T; L^1(\Omega))$. The inequality (1.66) also implies strong convergence of $\{\rho^{\Delta t,-}\}_{\Delta t > 0}$ in $L^1(0, T; L^1(\Omega))$ to $\widehat{\rho}$. This completes the proof of (1.65a) for $p = 1$.

From (1.61) we have that

$$\|\rho^{\Delta t,(\pm)}(t)\|_{L^1(\Omega)} \leq |\Omega|$$

for a.e. $t \in (0, T]$. This means that the sequences $\{\rho^{\Delta t,(\pm)}\}_{\Delta t > 0}$ are bounded in $L^\infty(0, T; L^1(\Omega))$. We can use Lemma 1.19 together with the strong convergence of the sequences $\{\rho^{\Delta t,(\pm)}\}_{\Delta t > 0}$ to $\widehat{\rho}$ in $L^1(0, T; L^1(\Omega))$ to deduce that we have strong convergence in $L^p(0, T; L^1(\Omega))$ to the same limit for all values of $p \in [1, \infty)$. We have then completed the proof of (1.65a).

Because strong convergence in $L^p(0, T; L^1(\Omega))$ for $p \in [1, \infty)$ implies convergence almost everywhere on $\Omega \times (0, T]$ of a subsequence (not indicated), it follows from (1.61a) that $\widehat{\rho} \geq 0$ a.e. on $\Omega \times (0, T)$. By applying Fubini's theorem we have that

$$\int_{\Omega} |\rho^{\Delta t,(\pm)} - \widehat{\rho}| \, dx \rightarrow 0 \quad \text{as } \Delta t \rightarrow 0_+ \text{ for a.e. } t \in (0, T].$$

Hence we have by (1.61b) that

$$\frac{1}{|\Omega|} \int_{\Omega} \widehat{\rho}(t) \, dx = 1 \quad \text{for a.e. } t \in (0, T].$$

We shall now prove (1.65b). We notice that since $|\sqrt{c_1} - \sqrt{c_2}| \leq \sqrt{|c_1 - c_2|}$ for any two nonnegative real numbers c_1 and c_2 , the strong convergence (1.65a) directly implies that, as $\Delta t \rightarrow 0_+$,

$$\sqrt{\rho^{\Delta t,(\pm)}} \rightarrow \sqrt{\widehat{\rho}} \quad \text{strongly in } L^p(0, T; L^2(\Omega)) \quad \text{for all } p \in [1, \infty).$$

The bound on the third term on the left-hand side of (1.64) implies the existence of a subsequence (not indicated) and an element $G \in L^2(0, T; L^2(\Omega; \mathbb{R}^d))$ such that

$$\nabla \sqrt{\rho^{\Delta t,(\pm)}} \rightarrow G \quad \text{weakly in } L^2(0, T; L^2(\Omega; \mathbb{R}^d)).$$

We have therefore that, for a test function $\eta \in C([0, T]; C_0^\infty(\Omega; \mathbb{R}^d))$,

$$\int_0^T \int_{\Omega} G \cdot \eta \, dx \, dt \leftarrow - \int_0^T \int_{\Omega} \sqrt{\rho^{\Delta t,(\pm)}} \operatorname{div} \eta \, dx \, dt \rightarrow - \int_0^T \int_{\Omega} \sqrt{\widehat{\rho}} \operatorname{div} \eta \, dx \, dt.$$

Therefore we have the equality

$$\int_0^T \int_{\Omega} G \cdot \eta \, dx \, dt = - \int_0^T \int_{\Omega} \sqrt{\widehat{\rho}} \operatorname{div} \eta \, dx \, dt,$$

and this means that G is the distributional gradient of $\sqrt{\widehat{\rho}}$. As $G \in L^2(0, T; L^2(\Omega; \mathbb{R}^d))$ it follows that

$$G = \nabla \sqrt{\widehat{\rho}} \in L^2(0, T; L^2(\Omega; \mathbb{R}^d))$$

and hence (1.65b) has been proved.

The weak convergence result (1.65c) follows from the uniform bound on the last term on the left-hand side of (1.64) and the weak compactness of bounded balls in the Hilbert space $L^2(0, T; H^{-\beta}(\Omega))$.

The weak-* convergence result (1.65d) follows from the uniform bound (1.50) stated in Lemma 1.17, the weak-* compactness of bounded balls in the Banach space $L^\infty(0, T; L^\infty(\Omega))$, and the uniqueness of the weak limit.

The strong convergence result (1.65e) is a direct consequence of (1.65a) and the uniform bound (1.50) stated in Lemma 1.17, using Lemma 1.19.

With the convergence (1.65e) in place, (1.65f) follows directly from (A.3) and (A.13c); that is,

$$\int_0^T \|c^{\Delta t, (\pm)}(t) - \widehat{c}(t)\|_{\mathbb{H}_*^s(\Omega)}^p \, dt \leq C \int_0^T \|\rho^{\Delta t, (\pm)}(t) - \widehat{\rho}(t)\|_{L_*^s(\Omega)}^p \, dt$$

for all $p \in [1, \infty)$.

Let us now consider the $L^2(0, T; L^2(\Omega; \mathbb{R}^d))$ norm of $\nabla c^{\Delta t, +}$. By the stability result (A.5) we have

$$\begin{aligned} \int_0^T \int_{\Omega} |\nabla c^{\Delta t, +}|^2 \, dx \, dt &\leq C \int_0^T \int_{\Omega} |\nabla \rho^{\Delta t, +}|^2 \, dx \, dt = 4C \int_0^T \int_{\Omega} \rho^{\Delta t, +} \left| \nabla \sqrt{\rho^{\Delta t, +}} \right|^2 \, dx \, dt \\ &\leq 4C \sup_{t \in (0, T]} \|\rho^{\Delta t, +}\|_{L^\infty(\Omega)} \int_0^T \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t, +}} \right|^2 \, dx \, dt, \end{aligned}$$

and thanks to the uniform bound on the $L^\infty(0, T; L^\infty(\Omega))$ norm of $\rho^{\Delta t, +}$ from Lemma 1.17 and the bound on the third term on the left-hand side of (1.64) we have that the $L^2(0, T; L^2(\Omega; \mathbb{R}^d))$ norm of the gradient of $c^{\Delta t, +}$ is uniformly bounded and therefore $\nabla c^{\Delta t, +}$ converges weakly to an element, that we call H , as $\Delta t \rightarrow 0_+$. By the convergence (1.65f) in $L^p(0, T; L^2(\Omega))$ we have that $\nabla c^{\Delta t, \pm}$ converges strongly to $\nabla \widehat{c}$ in $L^2(0, T; H^{-1}(\Omega; \mathbb{R}^d))$, but then $\nabla \widehat{c}$ must coincide with H because of the uniqueness of the weak limit.

We now want to use the convergence results we have just proved to pass to the limit as $\Delta t \rightarrow 0_+$ in equation (1.30a). Throughout the argument we will consider test functions $\phi \in C^1([0, T]; C^\infty(\overline{\Omega}))$ such that $\phi(\cdot, T) = 0$. Note that the set of all such test functions is dense in the set of functions belonging to $W^{1,1}(0, T; H^\beta(\Omega))$ and vanishing at $t = T$ (in the sense of the

trace theorem in $W^{1,1}(0, T)$), which is continuously embedded in $L^2(0, T; H^\beta(\Omega))$; therefore the use of such test functions is fully justified for the purposes of our argument.

We begin by considering the first term in (1.51a) and use integration by parts with respect to t to deduce that

$$\int_0^T \int_\Omega \frac{\partial \rho^{\Delta t}}{\partial t} \phi \, dx \, dt = - \int_0^T \int_\Omega \rho^{\Delta t} \frac{\partial \phi}{\partial t} \, dx \, dt - \int_\Omega \rho^0 \phi|_{t=0} \, dx$$

for all $\phi \in C^1([0, T], C^\infty(\bar{\Omega}))$ such that $\phi(\cdot, T) = 0$. Moreover,

$$\lim_{\Delta t \rightarrow 0_+} \rho^0 = \rho_0 \quad \text{weakly in } L^2(\Omega).$$

Therefore using (1.65a) we immediately have that, as $\Delta t \rightarrow 0_+$,

$$\int_0^T \int_\Omega \frac{\partial \rho_L^{\Delta t}}{\partial t} \phi \, dx \, dt \rightarrow - \int_0^T \int_\Omega \hat{\rho} \frac{\partial \phi}{\partial t} \, dx \, dt - \int_\Omega \rho_0 \phi|_{t=0} \, dx.$$

The second term in (1.51a) will be dealt with by decomposing it as follows:

$$\begin{aligned} \int_0^T \int_\Omega \nabla \rho^{\Delta t, +} \cdot \nabla \phi \, dx \, dt &= \underbrace{2 \int_0^T \int_\Omega \left(\sqrt{\rho^{\Delta t, +}} - \sqrt{\hat{\rho}} \right) \nabla \sqrt{\rho^{\Delta t, +}} \cdot \nabla \phi \, dx \, dt}_{\textcircled{1}} \\ &\quad + \underbrace{2 \int_0^T \int_\Omega \sqrt{\hat{\rho}} \nabla \sqrt{\rho^{\Delta t, +}} \cdot \nabla \phi \, dx \, dt}_{\textcircled{2}}. \end{aligned}$$

For term $\textcircled{1}$ we have by Hölder's inequality that

$$\begin{aligned} |\textcircled{1}| &\leq 2 \int_0^T \left(\int_\Omega \left| \sqrt{\rho^{\Delta t, +}} - \sqrt{\hat{\rho}} \right|^2 \, dx \right)^{\frac{1}{2}} \left(\int_\Omega \left| \nabla \sqrt{\rho^{\Delta t, +}} \right|^2 \, dx \right)^{\frac{1}{2}} \|\nabla \phi\|_{L^\infty(\Omega)} \, dt \\ &\leq 2 \left(\int_0^T \int_\Omega \left| \nabla \sqrt{\rho^{\Delta t, +}} \right|^2 \, dx \, dt \right)^{\frac{1}{2}} \left(\int_0^T \left\| \sqrt{\rho^{\Delta t, +}} - \sqrt{\hat{\rho}} \right\|_{L^2(\Omega)}^r \, dt \right)^{\frac{1}{r}} \\ &\quad \times \left(\int_0^T \|\nabla \phi\|_{L^\infty(\Omega)}^{\frac{2r}{r-2}} \, dt \right)^{\frac{r-2}{2r}}, \end{aligned}$$

where $r \in (2, \infty)$. Using the bound on the third term in the inequality stated in (1.64) we have

$$\begin{aligned} |\textcircled{1}| &\leq 2C_\star^{\frac{1}{2}} \left\| \sqrt{\rho^{\Delta t, +}} - \sqrt{\hat{\rho}} \right\|_{L^r(0, T; L^2(\Omega))} \|\nabla \phi\|_{L^{\frac{2r}{r-2}}(0, T; L^\infty(\Omega))} \\ &\leq 2C_\star^{\frac{1}{2}} \|\rho^{\Delta t, +} - \hat{\rho}\|_{L^{\frac{r}{2}}(0, T; L^1(\Omega))}^{\frac{1}{2}} \|\nabla \phi\|_{L^{\frac{2r}{r-2}}(0, T; L^\infty(\Omega))}, \end{aligned}$$

where we have used the elementary inequality $|\sqrt{c_1} - \sqrt{c_2}| \leq \sqrt{|c_1 - c_2|}$ with $c_1, c_2 \geq 0$. The first factor in the last line converges to 0 as $\Delta t \rightarrow 0_+$ thanks to (1.65a), and therefore the term $\textcircled{1}$ converges to 0 for every $\phi \in C^1([0, T]; C^\infty(\bar{\Omega}))$ as $\Delta t \rightarrow 0_+$.

Concerning the term ②, as $\hat{\rho} \in L^\infty(0, T; L^\infty(\Omega))$ and $\hat{\rho} \geq 0$ a.e. on $\Omega \times (0, T)$, we have that $\sqrt{\hat{\rho}} \nabla \phi$ belongs to $L^2(0, T; L^2(\Omega))$, and the weak convergence result (1.65b) then directly implies that

$$\begin{aligned} \lim_{\Delta t \rightarrow 0+} 2 \int_0^T \int_\Omega \sqrt{\hat{\rho}} \nabla \sqrt{\rho^{\Delta t, +}} \cdot \nabla \phi \, dx \, dt &= 2 \int_0^T \int_\Omega \sqrt{\hat{\rho}} \nabla \sqrt{\hat{\rho}} \cdot \nabla \phi \, dx \, dt \\ &= \int_0^T \int_\Omega \nabla \hat{\rho} \cdot \nabla \phi \, dx \, dt. \end{aligned}$$

Let us consider the final term in (1.51a). By (1.65e), $\rho^{\Delta t, +} \rightarrow \hat{\rho}$ strongly in $L^2(0, T; L^2(\Omega))$ and by (1.65g) $\nabla c^{\Delta t, +} \rightharpoonup \nabla \hat{c}$ weakly in $L^2(0, T; L^2(\Omega; \mathbb{R}^d))$; it follows that $\rho^{\Delta t, +} \nabla c^{\Delta t, +} \rightharpoonup \hat{\rho} \nabla \hat{c}$ weakly in $L^1(0, T; L^1(\Omega; \mathbb{R}^d))$, and therefore

$$\lim_{\Delta t \rightarrow 0+} \int_0^T \int_\Omega \rho^{\Delta t, +} \nabla c^{\Delta t, +} \cdot \nabla \phi \, dx \, dt = \int_0^T \int_\Omega \hat{\rho} \nabla \hat{c} \cdot \nabla \phi \, dx \, dt$$

for all $\phi \in C^1([0, T]; C^\infty(\overline{\Omega}))$.

Putting these convergence results together, and noting that $C^1([0, T]; C^\infty(\overline{\Omega}))$ is dense in the function space $W^{1,1}(0, T; H^\beta(\Omega))$ with $\beta = d + 1$, we get (1.65h).

Let us now prove the weak-* continuity of the function $\hat{\rho}$ as a map from $[0, T]$ to $L^\infty(\Omega)$. As $\hat{\rho} \in L^\infty(0, T; L^\infty(\Omega))$ and $\hat{\rho} \in H^1(0, T; H^{-\beta}(\Omega)) \subset C([0, T]; H^{-\beta}(\Omega))$, $\beta = d + 1$, and $L^\infty(\Omega) = L^1(\Omega)'$, it follows from part (b) of Lemma 1.20 with $X = L^\infty(\Omega)$, $Y = H^{-\beta}(\Omega)$ and $E = L^1(\Omega)$ that $\hat{\rho} \in C_{w*}([0, T]; L^\infty(\Omega))$. Because Ω is bounded, $L^\infty(\Omega) \subset L^1(\Omega)$, and it then directly follows from this weak-* continuity property of $\hat{\rho}$ that $\hat{\rho} \in C_w([0, T]; L^1(\Omega))$, i.e., $\hat{\rho}$ is weakly continuous as a mapping from $[0, T]$ to $L^1(\Omega)$.

It remains to prove the energy inequality (1.65i). Thanks to (1.59), in the form (1.60), and (1.29) we have that, for all $t \in (0, T]$,

$$\begin{aligned} \int_\Omega G(\rho^{\Delta t, +}(x, t)) \, dx - \frac{1}{2} \int_\Omega (\rho^{\Delta t, +})^*(x, t) c^{\Delta t, +}(x, t) \, dx \\ + \int_0^t \int_\Omega \left| 2 \nabla \sqrt{\rho^{\Delta t, +}} - \sqrt{\rho^{\Delta t, +}} \nabla c^{\Delta t, +} \right|^2 \, dx \, d\tau \\ \leq \int_\Omega G(\rho^0(x)) \, dx - \frac{1}{2} \int_\Omega (\rho^0)^*(x) c^0(x) \, dx \\ \leq \int_\Omega G(\rho_0(x)) \, dx - \frac{1}{2} \int_\Omega (\rho^0)^*(x) c^0(x) \, dx. \end{aligned} \tag{1.67}$$

Since G is a nonnegative, continuous and convex function, by [159, Proposition 7.7] and the strong convergence (1.65e) it follows that, for a.e. $t \in (0, T]$,

$$\int_\Omega G(\hat{\rho}(x, t)) \, dx \leq \liminf_{\Delta t \rightarrow 0+} \int_\Omega G(\rho^{\Delta t, +}(x, t)) \, dx. \tag{1.68}$$

As $\rho^0 = \rho^0(\Delta t)$ is uniformly bounded in $L^2(\Omega)$ with respect to $\Delta t > 0$, it follows that $(\rho^0)^*$ is uniformly bounded in $L_*^2(\Omega)$, and therefore by the continuous embedding of $L_*^2(\Omega) = \mathbb{H}_*^0(\Omega)$

into $\mathbb{H}_*^{-s}(\Omega)$, $(\rho^0)^*$ is uniformly bounded in $\mathbb{H}_*^{-s}(\Omega)$. By Theorem A.1, $c^0 = -(-\Delta_N)^{-s}(\rho^0)^*$ is then uniformly bounded in $\mathbb{H}^s(\Omega)$, and has therefore a weakly convergent subsequence (not indicated) in $\mathbb{H}^s(\Omega)$ as $\Delta t \rightarrow 0_+$; because $\mathbb{H}^s(\Omega)$ is compactly embedded in $\mathbb{H}^0(\Omega) = L^2(\Omega)$, we can extract a strongly convergent subsequence (not indicated) in $L^2(\Omega)$ as $\Delta t \rightarrow 0_+$. It remains to identify the limit of this subsequence. As $(\rho^0)^* \rightharpoonup (\rho_0)^*$ weakly in $L_*^2(\Omega)$ as $\Delta t \rightarrow 0_+$, thanks to the linearity of the operator $(-\Delta_N)^{-s}$, we have that $c^0 \rightharpoonup c_0 := -(-\Delta_N)^{-s}(\rho_0)^*$ weakly in $\mathbb{H}^s(\Omega)$, and therefore, thanks to the uniqueness of the weak limit $c^0 \rightarrow c_0 = -(-\Delta_N)^{-s}(\rho_0)^*$ strongly in $L^2(\Omega)$ as $\Delta t \rightarrow 0_+$. Hence, $(\rho^0)^* c^0 \rightharpoonup (\rho_0)^* c_0$ weakly in $L^1(\Omega)$ as $\Delta t \rightarrow 0_+$. Using this to pass to the limit in the second term on the right-hand side of the inequality (1.67) we have that

$$\lim_{\Delta t \rightarrow 0_+} \frac{1}{2} \int_{\Omega} (\rho^0)^*(x) c^0(x) dx = \frac{1}{2} \int_{\Omega} (\rho_0)^*(x) c_0(x) dx. \quad (1.69)$$

Concerning the second term on the left-hand side of (1.67), thanks to the strong convergence results (1.65e) and (1.65f) we have that $(\rho^{\Delta t,+})^* c^{\Delta t,+} \rightarrow (\hat{\rho})^* \hat{c}$, strongly in $L^1(0, T; L^1(\Omega))$, and therefore also,

$$\frac{1}{2} \int_{\Omega} (\rho^{\Delta t,+})^*(x, \cdot) c^{\Delta t,+}(x, \cdot) dx \rightarrow \frac{1}{2} \int_{\Omega} (\hat{\rho})^*(x, \cdot) \hat{c}(x, \cdot) dx$$

in $L^1(0, T)$ as $\Delta t \rightarrow 0_+$. Thus, for a subsequence (not indicated),

$$\frac{1}{2} \int_{\Omega} (\rho^{\Delta t,+})^*(x, t) c^{\Delta t,+}(x, t) dx \rightarrow \frac{1}{2} \int_{\Omega} (\hat{\rho})^*(x, t) \hat{c}(x, t) dx \quad (1.70)$$

for a.e. $t \in (0, T]$ as $\Delta t \rightarrow 0_+$.

Finally, for the third term on the left-hand side of (1.67) we use [107, Theorem 7.5] for the functional

$$u \mapsto \mathcal{J}(u) = \int_0^t \int_{\Omega} |u|^2 dx d\tau,$$

with respect to the sequence $2\nabla \sqrt{\rho^{\Delta t,+}} - \sqrt{\rho^{\Delta t,+}} \nabla c^{\Delta t,+}$ which can be equivalently written as $2\nabla \sqrt{\rho^{\Delta t,+}} + \sqrt{\rho^{\Delta t,+}} \nabla (-\Delta_N)^{-s}(\rho^{\Delta t,+})^*$, which is weakly convergent in $L^2(0, T; L^2(\Omega; \mathbb{R}^d))$ (identified with $L^2((0, T) \times \Omega; \mathbb{R}^2)$) to $2\nabla \sqrt{\hat{\rho}} - \sqrt{\hat{\rho}} \nabla \hat{c}$ by (1.65b), (1.65e) and (1.65g). The functional $\mathcal{J}(u)$ is clearly convex and therefore we have

$$\int_0^t \int_{\Omega} \left| 2\nabla \sqrt{\hat{\rho}} - \sqrt{\hat{\rho}} \nabla \hat{c} \right|^2 dx d\tau \leq \liminf_{\Delta t \rightarrow 0_+} \int_0^t \int_{\Omega} \left| 2\nabla \sqrt{\rho^{\Delta t,+}} - \sqrt{\rho^{\Delta t,+}} \nabla c^{\Delta t,+} \right|^2 dx d\tau. \quad (1.71)$$

Therefore, by inserting (1.68), (1.69), (1.70) and (1.71) into (1.67), we deduce that

$$\begin{aligned} \int_{\Omega} G(\hat{\rho}(x, t)) dx - \frac{1}{2} \int_{\Omega} (\hat{\rho})^*(x, t) \hat{c}(x, t) dx + \int_0^t \int_{\Omega} \left| 2\nabla \sqrt{\hat{\rho}} - \sqrt{\hat{\rho}} \nabla \hat{c} \right|^2 dx d\tau \\ \leq \int_{\Omega} G(\rho_0(x)) dx - \frac{1}{2} \int_{\Omega} (\rho_0)^*(x) c_0(x) dx \end{aligned}$$

for a.e. $t \in (0, T]$. Thus we have shown that

$$E(\hat{\rho}(t)) + \int_0^t \int_{\Omega} \left| 2\nabla \sqrt{\hat{\rho}} - \sqrt{\hat{\rho}} \nabla \hat{c} \right|^2 dx d\tau \leq E(\rho_0)$$

for a.e. $t \in (0, T]$ and the final result (1.65i) then directly follows. $\square$

As a conclusion of our argument in this section, we shall prove that the function $\widehat{\rho}$, which we defined via the limiting procedure detailed in Theorem 1.21, decays exponentially in time to the trivial solution of problem (1.4). As a consequence of this we shall also be able to strengthen the bound asserted in (1.65i); in particular we shall show that, provided that Ω is a bounded convex (and therefore Lipschitz) polytopal domain in $\mathbb{R}^d$, $d \in \{2, 3\}$, and $s \in (1/2, 1)$, the function $t \in [0, T] \mapsto E(\widehat{\rho}(t)) \in \mathbb{R}_{\geq 0}$ exhibits exponential decay. Extending the proof of exponential decay of the energy to $s \in (0, 1)$ constitutes an open problem and a potential direction for future work.

Let us first discuss a logarithmic Sobolev inequality, suitable for our purposes.

Lemma 1.22. *Let $f \in H^1(\Omega)$ be a nonnegative function. Then*

$$\int_{\Omega} f \log \left(\frac{f}{\frac{1}{|\Omega|} \int_{\Omega} f \, dx} \right) dx \leq 2C_{LS} \int_{\Omega} |\nabla \sqrt{f}|^2 dx, \quad (1.72)$$

with C_{LS} such that

$$C_{LS} \geq \frac{1}{\lambda_1}, \quad (1.73)$$

with λ_1 the first positive eigenvalue of the Neumann Laplacian.

Proof. The result is a consequence of the theory on logarithmic Sobolev inequalities and spectral gaps and we refer to [116] for a broader discussion on the topic.

The inequality (1.72) is known to hold on bounded Lipschitz domains; see, for example, [2, Theorem 1] and [2, Proposition 2.1 and Theorem 1]). Using the terminology of [116, Theorem 4.1] (1.72) is a logarithmic Sobolev inequality.

We have the Poincaré inequality

$$\int_{\Omega} \left(f - \frac{1}{|\Omega|} \int_{\Omega} f \, dx \right)^2 dx \leq C_{\Omega} \int_{\Omega} |\nabla f|^2 dx.$$

We note in passing that $C_{\Omega} = 1/\lambda_1$, with λ_1 the first positive eigenvalue of the Neumann Laplacian. Using the terminology of [116, Definition 2.1], the Poincaré inequality can be seen as a spectral gap inequality with constant $1/C_{\Omega}$ as spectral gap.

Finally using [116, Theorem 4.9] we have (1.73). $\square$

Theorem 1.23. *Suppose that the assumptions of Theorem 1.21 hold. Then, the weak solution $\widehat{\rho}$ we have constructed exhibits the following exponential decay properties.*

- (a) *For any $T > 0$, the functional $G(\cdot)$, defined in (1.9), exhibits exponential decay in the sense that*

$$\int_{\Omega} G(\widehat{\rho}(T)) \, dx \leq e^{-\frac{2T}{C_{LS}}} \int_{\Omega} G(\rho_0) \, dx, \quad (1.74)$$

where C_{LS} is a positive constant depending only on the domain Ω .

(b) The function $\widehat{\rho}$ satisfies the inequality

$$\frac{1}{2|\Omega|} \|\widehat{\rho}(\cdot, T) - 1\|_{L^1(\Omega)}^2 \leq e^{-\frac{2T}{C_{LS}}} E(\rho_0). \quad (1.75)$$

(c) Assuming in addition that $s \in (1/2, 1)$, the energy functional $E(\cdot)$, defined in (1.10), exhibits exponential decay for any $T > 0$, that is,

$$E(\widehat{\rho}(T)) \leq e^{-\frac{8T}{4C_{LS} + C_{\Omega, s} \|\rho_0\|_{L^\infty(\Omega)}}} E(\rho_0), \quad (1.76)$$

where $C_{\Omega, s} = 1/\lambda_1^{1+s}$, and λ_1 is the smallest positive eigenvalue of the Neumann Laplacian on the domain Ω .

Proof. (a) We start by taking $t = t_1 = \Delta t$ and $0 = t_0$ in (1.53). We have that, by definition, $\rho^0 = \rho^{\Delta t, -}(t_1)$. We adopt the notation $t_{-1} = -\infty$ in order to write $\rho^{\Delta t, +}(t_0)$ instead of $\rho^{\Delta t, -}(t_1)$. Therefore we have that

$$\int_{\Omega} G(\rho^{\Delta t, +}(t_1)) \, dx + \frac{1}{2\Delta t \|\rho_0\|_{L^\infty(\Omega)}} \int_{t_0}^{t_1} \int_{\Omega} (\rho^{\Delta t, +} - \rho^{\Delta t, -})^2 \, dx \, d\tau \quad (1.77)$$

$$\begin{aligned} &+ 4 \int_{t_0}^{t_1} \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t, +}} \right|^2 \, dx \, d\tau - \int_{t_0}^{t_1} \int_{\Omega} \nabla c^{\Delta t, +} \cdot \nabla \rho^{\Delta t, +} \, dx \, d\tau \\ &\leq \int_{\Omega} G(\rho^{\Delta t, +}(t_0)) \, dx. \end{aligned} \quad (1.78)$$

We can now repeat the argument that gave us (1.78) on each interval $[t_{n-1}, t_n]$ for $n = 1, \dots, N$, resulting in

$$\begin{aligned} &\int_{\Omega} G(\rho^{\Delta t, +}(t_n)) \, dx + \frac{1}{2\Delta t \|\rho_0\|_{L^\infty(\Omega)}} \int_{t_{n-1}}^{t_n} \int_{\Omega} (\rho^{\Delta t, +} - \rho^{\Delta t, -})^2 \, dx \, d\tau \\ &+ 4 \int_{t_{n-1}}^{t_n} \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t, +}} \right|^2 \, dx \, d\tau - \int_{t_{n-1}}^{t_n} \int_{\Omega} \nabla c^{\Delta t, +} \cdot \nabla \rho^{\Delta t, +} \, dx \, d\tau \\ &\leq \int_{\Omega} G(\rho^{\Delta t, +}(t_{n-1})) \, dx. \end{aligned} \quad (1.79)$$

We discard the nonnegative second term on the left-hand side of (1.79) to find that

$$\begin{aligned} &\int_{\Omega} G(\rho^{\Delta t, +}(t_n)) \, dx + 4 \int_{t_{n-1}}^{t_n} \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t, +}} \right|^2 \, dx \, d\tau - \int_{t_{n-1}}^{t_n} \int_{\Omega} \nabla c^{\Delta t, +} \cdot \nabla \rho^{\Delta t, +} \, dx \, d\tau \\ &\leq \int_{\Omega} G(\rho^{\Delta t, +}(t_{n-1})) \, dx. \end{aligned} \quad (1.80)$$

On a convex domain, for $t \in [t_{n-1}, t_n]$, $n = 1, \dots, N$, we can use the logarithmic Sobolev inequality (1.72) for the measure $d\mu(x) := \frac{1}{|\Omega|} \, dx$

$$\int_{\Omega} \rho^{\Delta t, +}(t) \log \rho^{\Delta t, +}(x, t) \, dx \leq 2C_{LS} \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t, +}(x, t)} \right|^2 \, dx,$$

with a positive constant $C_{LS} > 0$ depending only on the domain Ω . As $r \log r = G(r) - (1 - r)$, we can rewrite the above inequality as

$$\int_{\Omega} G(\rho^{\Delta t,+}(x, t)) \, dx \leq 2C_{LS} \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t,+}(x, t)} \right|^2 \, dx + \int_{\Omega} (1 - \rho^{\Delta t,+}(x, t)) \, dx$$

for $t \in (t_{n-1}, t_n]$, $n = 1, \dots, N$. Thanks to the fact that, by definition, $\rho^{\Delta t,+}$ is constant on the interval $(t_{n-1}, t_n]$ and (1.61b) holds, this implies that

$$\Delta t \int_{\Omega} G(\rho^{\Delta t,+}(x, t_n)) \, dx \leq 2C_{LS} \int_{t_{n-1}}^{t_n} \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t,+}(x, \tau)} \right|^2 \, dx \, d\tau \quad (1.81)$$

for $n = 1, \dots, N$. Using (1.80) and (1.81) we then have the inequality

$$\begin{aligned} \left(1 + \frac{2\Delta t}{C_{LS}}\right) \int_{\Omega} G(\rho^{\Delta t,+}(x, t_n)) \, dx - \int_{t_{n-1}}^{t_n} \int_{\Omega} \nabla c^{\Delta t,+} \cdot \nabla \rho^{\Delta t,+} \, dx \, d\tau \\ \leq \int_{\Omega} G(\rho^{\Delta t,+}(x, t_{n-1})) \, dx. \end{aligned} \quad (1.82)$$

For the sake of simplicity of the exposition we introduce the following notation:

$$\gamma := \frac{2}{C_{LS}}, \quad A_n := \int_{\Omega} G(\rho^{\Delta t,+}(t_n)) \, dx, \quad B_n := \int_{t_{n-1}}^{t_n} \int_{\Omega} \nabla c^{\Delta t,+} \cdot \nabla \rho^{\Delta t,+} \, dx \, d\tau.$$

We have that A_n is nonnegative. In terms of the new notation (1.82) can be rewritten as

$$(1 + \gamma\Delta t)A_n - B_n \leq A_{n-1}, \quad n = 1, \dots, N,$$

and therefore by induction we have that

$$A_n - \sum_{j=1}^n (1 + \gamma\Delta t)^{j-n-1} B_j \leq (1 + \gamma\Delta t)^{-n} A_0, \quad n = 1, \dots, N.$$

By the fact that $-B_j$ are nonnegative terms, we have

$$A_n - (1 + \gamma\Delta t)^{-n-1} \sum_{j=1}^n B_j \leq (1 + \gamma\Delta t)^{-n} A_0, \quad n = 1, \dots, N.$$

In particular, with $n = N$ we have

$$\begin{aligned} \int_{\Omega} G(\rho^{\Delta t,+}(x, T)) \, dx - (1 + \gamma\Delta t)^{-N-1} \int_0^T \int_{\Omega} \nabla c^{\Delta t,+} \cdot \nabla \rho^{\Delta t,+} \, dx \, d\tau \\ \leq (1 + \gamma\Delta t)^{-N} \int_{\Omega} G(\rho^{\Delta t,+}(x, 0)) \, dx. \end{aligned}$$

We recall that $\rho^{\Delta t,+}(0) = \rho^0$ and thus we arrive at the following inequality:

$$\begin{aligned} \int_{\Omega} G(\rho^{\Delta t,+}(x, T)) \, dx - \left(1 + \frac{2\Delta t}{C_{LS}}\right)^{-N-1} \int_0^T \int_{\Omega} \nabla c^{\Delta t,+} \cdot \nabla \rho^{\Delta t,+} \, dx \, d\tau \\ \leq \left(1 + \frac{2\Delta t}{C_{LS}}\right)^{-N} \int_{\Omega} G(\rho^0) \, dx \\ \leq \left(1 + \frac{2\Delta t}{C_{LS}}\right)^{-N} \int_{\Omega} G(\rho_0) \, dx. \end{aligned} \quad (1.83)$$

We first discard the (nonnegative) second term on the left-hand side of (1.83) recalling (1.54). It then remains to pass to the limit in the resulting inequality as $\Delta t \rightarrow 0_+$. Before doing so, we need make a few additional technical observations.

Thanks to (1.65a) we have that, on passing to a subsequence, $\rho^{\Delta t}(T)$ converges weakly to $\widehat{\rho}(T)$ in $H^{-\beta}(\Omega)$ with $\beta = d + 1$ as $\Delta t \rightarrow 0_+$. Noting the bound on the first term of (1.64) and that $G(r)/r \rightarrow +\infty$ as $r \rightarrow +\infty$, we deduce from de la Vallée-Poussin's theorem that the family $\{\rho^{\Delta t}(T)\}_{\Delta t > 0}$ is uniformly integrable in $L^1(\Omega)$. Hence, by the Dunford–Pettis theorem, $\{\rho^{\Delta t}(T)\}_{\Delta t > 0}$ is weakly relatively compact in $L^1(\Omega)$. Consequently, upon extraction of a further subsequence (not indicated), $\rho^{\Delta t}(T)$ converges weakly in $L^1(\Omega)$ to some limit as $\Delta t \rightarrow 0_+$; however the uniqueness of the weak limit together with the weak convergence of the sequence in $H^{-\beta}(\Omega)$, $\beta = d + 1$, implies that the sequence $\rho^{\Delta t}(T)$ converges to $\widehat{\rho}(T)$ weakly in $L^1(\Omega)$, because $L^1(\Omega)$ is continuously embedded in $H^{-\beta}(\Omega)$ for $\beta = d + 1$. Finally, since the function G is continuous and convex, by applying Tonelli's semicontinuity theorem in $L^1(\Omega)$,

$$\int_{\Omega} G(\widehat{\rho}(x, T)) \, dx \leq \liminf_{\Delta t \rightarrow 0_+} \int_{\Omega} G(\rho^{\Delta t, +}(x, T)) \, dx, \quad (1.84)$$

by noticing that $\rho^{\Delta t, +}(x, T) = \rho^{\Delta t}(x, T)$ for a.e. $x \in \Omega$. We can now pass to the limit as $\Delta t \rightarrow 0_+$ (with $N = T/\Delta t \rightarrow +\infty$) in (1.83), using (1.65a) and (1.84); hence we find that

$$\int_{\Omega} G(\widehat{\rho}(x, T)) \, dx \leq e^{-\frac{2T}{c_{LS}}} \int_{\Omega} G(\rho_0(x)) \, dx, \quad (1.85)$$

which proves part (a).

(b) The Csiszár–Kullback inequality [169], with the probability measure $d\mu(x) := \frac{1}{|\Omega|} dx$ on Ω , yields that

$$\int_{\Omega} |\widehat{\rho}(x, T) - 1| \, d\mu(x) \leq \left(2 \int_{\Omega} G(\widehat{\rho}(x, T)) \, d\mu(x) \right)^{\frac{1}{2}},$$

thanks to the fact that $\widehat{\rho}(x, t) \geq 0$ for a.e. $x \in \Omega$ and $\int_{\Omega} \widehat{\rho}(x, T) \, d\mu(x) = 1$, and therefore

$$\|\widehat{\rho}(\cdot, T) - 1\|_{L^1(\Omega)}^2 \leq 2|\Omega| \int_{\Omega} G(\widehat{\rho}(x, T)) \, dx.$$

Combining this with (1.85) finally gives the desired result (1.75) of part (b), by the fact that $\int_{\Omega} G(\rho_0) \, dx \leq E(\rho_0)$ for the energy functional $E(\cdot)$ defined in (1.10).

(c) We conclude by proving part (c) with the additional assumption that the fractional order s lies in between $\frac{1}{2}$ and 1. To this end, we shall focus on the second term in the expression (1.10) of the energy functional $E(\rho^{\Delta t, +})$, that is, on the interaction term between $\rho^{\Delta t, +}$ and $c^{\Delta t, +}$.

We notice that, from (1.57), taking $t = t_1$ and $0 = t_0$ as we did previously, we have

$$\begin{aligned} & \frac{1}{2} \int_{\Omega} (-\Delta_N)^s c^{\Delta t, +}(x, t_1) c^{\Delta t, +}(x, t_1) \, dx + \int_{t_0}^{t_1} \int_{\Omega} \rho^{\Delta t, +} |\nabla c^{\Delta t, +}|^2 \, dx \, d\tau \\ & - \int_{t_0}^{t_1} \int_{\Omega} \nabla \rho^{\Delta t, +} \cdot \nabla c^{\Delta t, +} \, dx \, d\tau \leq \frac{1}{2} \int_{\Omega} (-\Delta_N)^s c^{\Delta t, +}(x, t_0) c^{\Delta t, +}(x, t_0) \, dx, \end{aligned}$$

and then, on each interval $[t_{n-1}, t_n]$ for $n = 1, \dots, N$,

$$\begin{aligned} \frac{1}{2} \int_{\Omega} (-\Delta_N)^s c^{\Delta t, +}(x, t_n) c^{\Delta t, +}(x, t_n) dx &+ \int_{t_{n-1}}^{t_n} \int_{\Omega} \rho^{\Delta t, +} |\nabla c^{\Delta t, +}|^2 dx d\tau \\ &- \int_{t_{n-1}}^{t_n} \int_{\Omega} \nabla \rho^{\Delta t, +} \cdot \nabla c^{\Delta t, +} dx d\tau \\ &\leq \frac{1}{2} \int_{\Omega} (-\Delta_N)^s c^{\Delta t, +}(x, t_{n-1}) c^{\Delta t, +}(x, t_{n-1}) dx. \end{aligned} \quad (1.86)$$

For $t \in [t_{n-1}, t_n]$ with $n = 1, \dots, N$, by (A.3) and Poincaré's inequality we have that

$$\begin{aligned} \|c^{\Delta t, +}(t)\|_{\mathbb{H}^s(\Omega)}^2 &= \int_{\Omega} (-\Delta_N)^s c^{\Delta t, +}(x, t) c^{\Delta t, +}(x, t) dx \\ &\leq \tilde{C}_{\Omega, s} \int_{\Omega} ((\rho^{\Delta t, +})^*(x, t))^2 dx \\ &\leq \tilde{C}_{\Omega, s} C_{\Omega} \int_{\Omega} |\nabla (\rho^{\Delta t, +})^*(x, t)|^2 dx \\ &\leq \tilde{C}_{\Omega, s} C_{\Omega} \|\rho_0\|_{L^\infty(\Omega)} \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t, +}(x, t)} \right|^2 dx, \end{aligned}$$

where $\tilde{C}_{\Omega, s} = 1/\lambda_1^s$ and $C_{\Omega} = 1/\lambda_1$, with λ_1 the first positive eigenvalue of the Neumann Laplacian in Ω . Hence, denoting $C_{\Omega, s} = 1/\lambda_1^{1+s}$, we have

$$\Delta t \int_{\Omega} (-\Delta_N)^s c^{\Delta t, +}(x, t_n) c^{\Delta t, +}(x, t_n) dx \leq C_{\Omega, s} \|\rho_0\|_{L^\infty(\Omega)} \int_{t_{n-1}}^{t_n} \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t, +}(x, \tau)} \right|^2 dx d\tau. \quad (1.87)$$

We combine (1.81) and (1.87) to find the following inequality for the energy functional $E(\cdot)$:

$$\begin{aligned} \Delta t E(\rho^{\Delta t, +}(\cdot, t_n)) &= \Delta t \int_{\Omega} G(\rho^{\Delta t, +}(x, t_n)) dx \\ &+ \frac{1}{2} \Delta t \int_{\Omega} (-\Delta_N)^s c^{\Delta t, +}(x, t_n) c^{\Delta t, +}(x, t_n) dx \\ &\leq \frac{1}{2} (4C_{LS} + C_{\Omega, s} \|\rho_0\|_{L^\infty(\Omega)}) \int_{t_{n-1}}^{t_n} \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t, +}(x, \tau)} \right|^2 dx d\tau. \end{aligned} \quad (1.88)$$

By summing (1.80), (1.86) we also have that

$$\begin{aligned} E(\rho^{\Delta t, +}(\cdot, t_n)) &+ 4 \int_{t_{n-1}}^{t_n} \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t, +}} \right|^2 dx d\tau + \int_{t_{n-1}}^{t_n} \int_{\Omega} \rho^{\Delta t, +} |\nabla c^{\Delta t, +}|^2 dx d\tau \\ &- \int_{t_{n-1}}^{t_n} \int_{\Omega} \nabla c^{\Delta t, +} \cdot \nabla \rho^{\Delta t, +} dx d\tau \leq E(\rho^{\Delta t, +}(\cdot, t_{n-1})), \end{aligned}$$

and by (1.88) we deduce the following inequality:

$$\begin{aligned} \left(1 + \frac{8\Delta t}{4C_{LS} + C_{\Omega, s} \|\rho_0\|_{L^\infty(\Omega)}} \right) E(\rho^{\Delta t, +}(\cdot, t_n)) &+ \int_{t_{n-1}}^{t_n} \int_{\Omega} \rho^{\Delta t, +} |\nabla c^{\Delta t, +}|^2 dx d\tau \\ &- \int_{t_{n-1}}^{t_n} \int_{\Omega} \nabla c^{\Delta t, +} \cdot \nabla \rho^{\Delta t, +} dx d\tau \leq E(\rho^{\Delta t, +}(\cdot, t_{n-1})). \end{aligned} \quad (1.89)$$

Similarly as we did previously, we introduce the following auxiliary notation:

$$\begin{aligned}\delta &:= \frac{8}{4C_{LS} + C_{\Omega,s}\|\rho_0\|_{L^\infty(\Omega)}}, & C_n &:= E(\rho^{\Delta t,+}(x, t_n)), \\ D_n &:= \int_{t_{n-1}}^{t_n} \int_{\Omega} \rho^{\Delta t,+} \left| \nabla c^{\Delta t,+} \right|^2 dx d\tau - \int_{t_{n-1}}^{t_n} \int_{\Omega} \nabla c^{\Delta t,+} \cdot \nabla \rho^{\Delta t,+} dx d\tau.\end{aligned}$$

We have that C_n is nonnegative. In terms of this new notation (1.89) can be rewritten as

$$(1 + \delta\Delta t)C_n + D_n \leq C_{n-1}, \quad n = 1, \dots, N,$$

and therefore by induction and the fact that D_n is nonnegative we have that

$$C_n + (1 + \delta\Delta t)^{-n} \sum_{j=1}^n D_j \leq (1 + \delta\Delta t)^{-n} C_0, \quad n = 1, \dots, N.$$

In particular, with $n = N$ we have

$$\begin{aligned}E(\rho^{\Delta t,+}(\cdot, T)) + (1 + \delta\Delta t)^{-N} \int_0^T \int_{\Omega} \rho^{\Delta t,+} \left| \nabla c^{\Delta t,+} \right|^2 dx d\tau \\ - (1 + \delta\Delta t)^{-N} \int_0^T \int_{\Omega} \nabla c^{\Delta t,+} \cdot \nabla \rho^{\Delta t,+} dx d\tau \\ \leq (1 + \delta\Delta t)^{-N} E(\rho^{\Delta t,+}(\cdot, 0)).\end{aligned}$$

We recall that $\rho^{\Delta t,+}(0) = \rho^0$ and thus we arrive at the following inequality:

$$\begin{aligned}E(\rho^{\Delta t,+}(\cdot, T)) + \left(1 + \frac{8\Delta t}{4C_{LS} + C_{\Omega,s}\|\rho_0\|_{L^\infty(\Omega)}}\right)^{-N} \int_0^T \int_{\Omega} \rho^{\Delta t,+} \left| \nabla c^{\Delta t,+} \right|^2 dx d\tau \\ - \left(1 + \frac{8\Delta t}{4C_{LS} + C_{\Omega,s}\|\rho_0\|_{L^\infty(\Omega)}}\right)^{-N} \int_0^T \int_{\Omega} \nabla c^{\Delta t,+} \cdot \nabla \rho^{\Delta t,+} dx d\tau \\ \leq \left(1 + \frac{8\Delta t}{4C_{LS} + C_{\Omega,s}\|\rho_0\|_{L^\infty(\Omega)}}\right)^{-N} E(\rho^0).\end{aligned} \tag{1.90}$$

We first discard the (nonnegative) second and third terms on the left-hand side of (1.90) recalling (1.54). It then remains to pass to the limit in the resulting inequality as $\Delta t \rightarrow 0_+$. We use the argument that allowed us to pass to the limit before and prove (1.85), together with additional considerations for the interaction term involved in the energy functional.

We begin by noting that

$$\begin{aligned}(\rho^{\Delta t})^*(x, t) &:= \rho^{\Delta t}(x, t) - \frac{1}{|\Omega|} \int_{\Omega} \rho^{\Delta t}(\xi, t) d\xi = \rho^{\Delta t}(x, t) - \frac{1}{|\Omega|} \int_{\Omega} \rho^{\Delta t}(\xi, 0) d\xi \\ &= \rho^{\Delta t}(x, t) - \frac{1}{|\Omega|} \int_{\Omega} \rho^0(\xi) d\xi = \rho^{\Delta t}(x, t) - \frac{1}{|\Omega|} \int_{\Omega} \rho_0(\xi) d\xi = \rho^{\Delta t}(x, t) - 1.\end{aligned}$$

Hence,

$$\frac{\partial(\rho^{\Delta t})^*}{\partial t} = \frac{\partial \rho^{\Delta t}}{\partial t}.$$

Because $c^{\Delta t} = -(-\Delta_N)^{-s}(\rho^{\Delta t})^*$ and $c^{\Delta t}$ and $(\rho^{\Delta t})^*$ are continuous piecewise linear functions of $t \in [0, T]$ on the partition $0 = t_0 < t_1 < \dots < t_N = T$, it follows from the linearity of the differential operator $-(-\Delta_N)^{-s}$ and its independence of t that

$$\frac{\partial c^{\Delta t}}{\partial t} = -(-\Delta_N)^{-s} \frac{\partial (\rho^{\Delta t})^*}{\partial t} = -(-\Delta_N)^{-s} \frac{\partial \rho^{\Delta t}}{\partial t}.$$

Thereby, for any function $\phi \in W^{1,\infty}(\Omega)$, we have that

$$\begin{aligned} \left| \int_0^T \int_{\Omega} \frac{\partial c^{\Delta t}}{\partial t} \phi \, dx \, dt \right| &= \left| \int_0^T \int_{\Omega} \frac{\partial c^{\Delta t}}{\partial t} \phi^* \, dx \, dt \right| = \left| \int_0^T \int_{\Omega} (-\Delta_N)^{-s} \frac{\partial \rho^{\Delta t}}{\partial t} \phi^* \, dx \, dt \right| \\ &= \left| \int_0^T \int_{\Omega} \frac{\partial \rho^{\Delta t}}{\partial t} (-\Delta_N)^{-s} \phi^* \, dx \, dt \right| \\ &\leq C_{\star} \left(\int_0^T \|(-\Delta_N)^{-s} \phi^*\|_{W^{1,\infty}(\Omega)}^2 \, dt \right)^{\frac{1}{2}} \\ &\leq C_{\star} \left(\int_0^T \|\phi^*\|_{L^{\infty}(\Omega)}^2 \, dt \right)^{\frac{1}{2}} \leq C_{\star} \left(\int_0^T \|\phi^*\|_{W^{1,\infty}(\Omega)}^2 \, dt \right)^{\frac{1}{2}}, \end{aligned} \quad (1.91)$$

where in the first equality of the first line we used the fact that, by definition, $c^{\Delta t}$ has zero integral average over Ω and therefore the same is true of its time-derivative; in the equality appearing in the second line we used the selfadjointness of $(-\Delta_N)^{-s}$ on $L_*^2(\Omega)$, and in the inequality appearing in the third line we made use of the first inequality in (1.62); and in the passage from the third to the fourth line we used Lemma A.9, which requires the assumption on the convexity of Ω and the restriction on the fractional order s to the range $s \in (1/2, 1)$.

Hence, thanks to the fact that $H^2(\Omega)$ is continuously embedded in $L^{\infty}(\Omega)$ for $d = 2, 3$, we deduce from (1.91) the following uniform bound on the time-derivative of $c^{\Delta t}$ in $L^2(0, T; H^{-2}(\Omega))$, where $H^{-2}(\Omega) := [H^2(\Omega)]'$:

$$\left| \int_0^T \int_{\Omega} \frac{\partial c^{\Delta t}}{\partial t} \phi \, dx \, dt \right| \leq C_{\star} \left(\int_0^T \|\phi\|_{H^2(\Omega)}^2 \, dt \right)^{\frac{1}{2}},$$

for all $\phi \in H^2(\Omega)$, where $C_{\star}$ is a positive constant, independent of ϕ and Δt . Using the weak compactness of bounded balls in the Hilbert space $L^2(0, T; H^{-2}(\Omega))$ we then have that

$$\frac{\partial c^{\Delta t}}{\partial t} \rightharpoonup \frac{\partial \widehat{c}}{\partial t} \quad \text{weakly in } L^2(0, T; H^{-2}(\Omega)).$$

By Lemma A.9, combined with the fact that $\rho^{\Delta t} \in L^{\infty}(0, T; L^{\infty}(\Omega))$ and is uniformly bounded with respect to Δt in the norm of $L^{\infty}(0, T; L^{\infty}(\Omega))$ and the fact that $\widehat{\rho} \in L^{\infty}(0, T; L^{\infty}(\Omega))$ we have, respectively, that $c^{\Delta t} \in L^{\infty}(0, T; W^{1,\infty}(\Omega))$ and is uniformly bounded with respect to Δt in the norm of $L^{\infty}(0, T; W^{1,\infty}(\Omega))$ and $\widehat{c} \in L^{\infty}(0, T; W^{1,\infty}(\Omega))$. Hence by the Aubin–Lions lemma $\{c^{\Delta t}\}_{\Delta t > 0}$ is compact in $C([0, T]; X)$ for any Banach space X such that $W^{1,\infty}(\Omega) \hookrightarrow X \hookrightarrow H^{-2}(\Omega)$; in particular, (upon extraction of a subsequence, not indicated) $c^{\Delta t}$ converges to

$\widehat{c}$ strongly in $C([0, T]; L^\infty(\Omega))$. As $\widehat{\rho} \in C_w^*([0, T]; L^\infty(\Omega))$, it then follows that the product $\widehat{\rho}\widehat{c}$ belongs to $C_w^*([0, T]; L^\infty(\Omega))$, and therefore also to $C_w([0, T]; L^1(\Omega))$; in particular,

$$t \in [0, T] \mapsto \int_{\Omega} \widehat{\rho}(x, t) \widehat{c}(x, t) \, dx \in \mathbb{R}$$

is a continuous function. Furthermore, because $\rho^{\Delta t}(T) \rightharpoonup \widehat{\rho}(T)$ weakly in $L^1(\Omega)$ and $c^{\Delta t}(T) \rightarrow \widehat{c}(T)$ strongly in $L^\infty(\Omega)$ as $\Delta t \rightarrow 0_+$, it follows that $\rho^{\Delta t}(T) c^{\Delta t}(T) \rightharpoonup \widehat{\rho}(T) \widehat{c}(T)$ weakly in $L^1(\Omega)$ as $\Delta t \rightarrow 0_+$. Thus we deduce that

$$\lim_{\Delta t \rightarrow 0_+} \int_{\Omega} \rho^{\Delta t}(x, T) c^{\Delta t}(x, T) \, dx = \int_{\Omega} \widehat{\rho}(x, T) \widehat{c}(x, T) \, dx. \quad (1.92)$$

We can now pass to the limit as $\Delta t \rightarrow 0_+$ (with $N = T/\Delta t \rightarrow +\infty$) in (1.90), using (1.84), and (1.92). Hence we find that

$$E(\widehat{\rho}(\cdot, T)) \leq e^{-\frac{8T}{4C_{LS} + C_{\Omega, s} \|\rho_0\|_{L^\infty(\Omega)}}} E(\rho_0).$$

This completes the proof. □

*Ma non piegato insino allora indarno
Codardamente supplicando innanzi
Al futuro oppressor; ma non eretto
Con forsennato orgoglio inver le stelle*

Giacomo Leopardi (1798-1837), “La ginestra”

2

A minimax method for the spectral fractional Laplacian

We now move on to discuss some of the computational aspects of the numerical method that we have described in Chapter 1. In particular we will devote large part of the chapter to developing an efficient algorithm to compute the finite element approximation of the spectral fractional Laplacian. The use of the discrete spectral fractional Laplacian (1.20) a priori assumes full knowledge of the discrete set of eigenvalues $\lambda_1^h, \dots, \lambda_{N_h-1}^h$, which is clearly computationally expensive as h decreases. The algorithm that we will discuss has the advantage of not needing the whole discrete spectrum, but only a lower and upper bound for the interval containing the eigenvalues. As we highlighted in the Introduction, the scientific novelty of this chapter does not lie in the algorithm itself, but in its application and its integration with a state-of-the-art finite element software to compute the approximations of the evolutionary nonlocal PDEs that are the focus of our work. Thus, after the description of the method, we will perform numerical simulations for nonlocal evolutionary problems, such as the fractional porous medium equation discussed in Chapter 1.

Even though for our purposes the algorithm serves as an efficient tool to obtain approximations for the problems of interest, its description stands by its own as regards the computation of the fractional Laplacian in elliptic problems of the type (17), i.e. fractional Poisson equations. Therefore, we will first introduce the algorithm for computing a finite element approximation of the spectral fractional Laplacian to solve elliptic problems, with its computational validation in conjunction with the associated error estimates in one and two dimensions for different fractional orders. We have not found in the literature such a complete validation of this type of method, specifically in two dimensions. We will then proceed to use the algorithm for our time-dependent

model, in order to numerically validate some of the properties of the fractional porous medium equation and a related PDE, that is the fractional Keller–Segel model.

Let us therefore consider the spectral fractional Laplacian with a generic boundary condition $\mathcal{B}(\cdot)$ that we first introduced in (12), which can be a Neumann boundary condition (as the one set in (1.4)) or a Dirichlet boundary condition (this will be the case for the Keller–Segel model as we will discuss later). Hence, we study the general fractional Poisson equation

$$(-\Delta_{\mathcal{B}})^s u = f \quad \text{in } \Omega, \quad \mathcal{B}(u) = 0 \quad \text{on } \partial\Omega. \quad (2.1)$$

More generally with respect to Chapter 1, we can define a space V that coincides with $H_0^1(\Omega)$ in the case of a Dirichlet boundary condition and that coincides with $H_*^1(\Omega)$ in the case of a Neumann boundary condition. In this general setting, if we consider a triangulation $\mathcal{T}_h$ as the one defined in Section 1.2, let V_h be the linear space consisting of all continuous piecewise affine functions defined on $\mathcal{T}_h$:

$$V_h := \{v_h \in C(\overline{\Omega}) \text{ such that } v_h|_K \in \mathbb{P}^1 \text{ for all } K \in \mathcal{T}_h\}, \quad (2.2)$$

and let N_h be its dimension, $N_h := \dim V_h$. Let us denote by $\{\phi_i\}_{i=1}^{N_h}$ the nodal basis of V_h , such that $\phi_i(P_j) = \delta_{i,j}$, where $\{P_j\}_{j=1}^{N_h}$ are the mesh points (vertices) of $\mathcal{T}_h$. Let $\mathcal{J}_h \subset \{1, \dots, N_h\}$ denote the following subset of indices,

$$\mathcal{J}_h := \begin{cases} \{j : P_j \in \Omega\} & \text{in case of a homogeneous Dirichlet boundary condition,} \\ \{1, \dots, N_h\} & \text{in case of a homogeneous Neumann boundary condition,} \end{cases}$$

and let $\mathcal{N}_h := |\mathcal{J}_h|$; in case of a Dirichlet boundary $\mathcal{J}_h$ are the indices of the interior vertices. Moreover let $\mathcal{I}_h : \mathbb{R}^{\mathcal{N}_h} \rightarrow V_h$ be the interpolation operator defined as

$$\mathcal{I}_h \mathbf{v} = \sum_{i \in \mathcal{J}_h} v_i \phi_i, \quad \text{for } \mathbf{v} \in \mathbb{R}^{\mathcal{N}_h}, \quad (2.3)$$

which takes a vector $\mathbf{v}$ in $\mathbb{R}^{\mathcal{N}_h}$ and maps it into the function $\mathcal{I}_h \mathbf{v}$ in V_h . Let us denote by $\mathcal{V}_h$ the space $\mathcal{V}_h := \text{span}\{\phi_i\}_{i \in \mathcal{J}_h}$ so that $\mathcal{V}_h = V_h \cap V (= V_h \cap H_0^1(\Omega))$ for a Dirichlet boundary and $\mathcal{V}_h = V_h$ in the Neumann case.

Let us consider the eigenvalue problem for the Laplacian, stated in its weak form:

$$\text{Find } \varphi \in V \setminus \{0\} \text{ and } \lambda \in \mathbb{R} \text{ such that } (\nabla \varphi, \nabla v) = \lambda(\varphi, v) \text{ for all } v \in V. \quad (2.4)$$

The finite element approximation of this eigenvalue problem is obtained by considering the restriction of the weak formulation (2.4) to the finite element space $V_h \cap V$:

$$\text{Find } \varphi_h \in V_h \cap V \setminus \{0\} \text{ and } \lambda^h \in \mathbb{R} \text{ such that } (\nabla \varphi_h, \nabla v_h) = \lambda^h(\varphi_h, v_h) \text{ for all } v_h \in V_h \cap V. \quad (2.5)$$

Similarly as in Section 1.2, we can define the discrete Laplacian $L_h : V_h \cap V \rightarrow V_h \cap V$ by the identity $(L_h w_h, v_h) := (\nabla w_h, \nabla v_h)$ for all $v_h \in V_h \cap V$. The linear operator L_h is positive and selfadjoint, and has a discrete set of eigenvalues $0 < \lambda_1^h \leq \lambda_2^h \leq \dots \leq \lambda_{\dim(V_h \cap V)}^h$, with corresponding eigenfunctions $\{\varphi_k^h\}_{k=1}^{\dim(V_h \cap V)}$, which form an orthonormal basis (with respect to the inner product $(\cdot, \cdot)$) for the space $V_h \cap V$. We notice that then for a Dirichlet boundary condition $\{\varphi_k^h\}_{k=1}^{\dim(V_h \cap V)}$ constitutes also a basis for $\mathcal{V}_h$ by definition of it; in fact $\dim(V_h \cap V) = \mathcal{N}_h$. In the case of a Neumann boundary condition $\dim(V_h \cap V) = \mathcal{N}_h - 1$ and thus, for later use, we introduce the function $\varphi_0^h = |\Omega|^{-1/2}$ that is an orthonormal eigenfunction with vanishing eigenvalue $\lambda_0^h = 0$. This allows us to define a discrete version of the spectral fractional Laplacian, as in (1.20),

$$(-\Delta_h)^s u_h = \sum_{k=1}^{\dim(V_h \cap V)} (\lambda_k^h)^s u_k^h \varphi_k^h, \quad \text{where } u_k^h = \int_{\Omega} u_h \varphi_k^h dx \quad \text{and } s \in (0, 1). \quad (2.6)$$

With these definitions in place, the finite element approximation of the fractional Poisson equation (2.1) is as follows:

$$\text{Find } u_h \in V_h \cap V \quad \text{such that} \quad ((-\Delta_h)^s u_h, v_h) = (f, v_h) \quad \text{for all } v_h \in V_h \cap V, \quad (2.7)$$

and it can be rewritten in the following equivalent form:

$$\text{Find } u_h \in V_h \quad \text{such that} \quad \sum_{k=1}^{\dim(V_h \cap V)} (\lambda_k^h)^s u_k^h (\varphi_k^h, v_h) = (f, v_h) \quad \text{for all } v_h \in V_h \cap V.$$

Since $\{\varphi_j^h\}_{j=1}^{\dim(V_h \cap V)}$ is an orthonormal basis for $V_h \cap V$ with respect to the inner product $(\cdot, \cdot)$, we have that

$$(\lambda_j^h)^s u_j^h = (f, \varphi_j^h) \quad \text{for all } j = 1, \dots, \dim(V_h \cap V). \quad (2.8)$$

As mentioned before, in the case of a Dirichlet boundary condition $\dim(V_h \cap V) = \mathcal{N}_h$ and thus $\Lambda \in \mathbb{R}^{\mathcal{N}_h \times \mathcal{N}_h}$. Therefore, in the case of a Dirichlet boundary condition, writing (2.8) as a linear system gives

$$\Lambda^s \tilde{U} = \tilde{F}, \quad \text{with } \tilde{U} = (u_1^h, \dots, u_{\mathcal{N}_h}^h)^T, \\ \tilde{F} = ((f, \varphi_1^h), \dots, (f, \varphi_{\mathcal{N}_h}^h))^T, \quad \Lambda = \text{diag}(\lambda_1^h, \dots, \lambda_{\mathcal{N}_h}^h).$$

For the Neumann boundary condition we add the constant eigenfunction defined previously, so that we can write

$$\Lambda^s \tilde{U} = \tilde{F}, \quad \text{with } \tilde{U} = (u_0^h, u_1^h, \dots, u_{\mathcal{N}_h-1}^h)^T, \\ \tilde{F} = ((f, \varphi_0^h), (f, \varphi_1^h), \dots, (f, \varphi_{\mathcal{N}_h-1}^h))^T, \quad \Lambda = \text{diag}(\lambda_0^h, \lambda_1^h, \dots, \lambda_{\mathcal{N}_h-1}^h).$$

Let X be the matrix of change of variables between $\{\varphi_j^h\}_j$ and the usual finite element basis $\{\phi_i\}_{i \in \mathcal{J}_h}$ such that $U = X\tilde{U}$ and $F = X\tilde{F}$. Then the linear system can be rewritten as

$$X\Lambda^s X^{-1}U = F, \quad (2.9)$$

where $F = \mathcal{M}^{-1}((f, \phi_i))_i^T$.

Lemma 2.1. *Let $\{\phi_i\}_{i=1}^{N_h}$ be the nodal basis of the space V_h defined in (2.2), and let $\mathcal{S} \in \mathbb{R}^{N_h \times N_h}$ and $\mathcal{M} \in \mathbb{R}^{N_h \times N_h}$ be the stiffness matrix and mass matrix, respectively, defined as follows: $\mathcal{S}_{i,j} = (\nabla \phi_i, \nabla \phi_j)$, $\mathcal{M}_{i,j} = (\phi_i, \phi_j)$, $i, j \in \mathcal{J}_h$. The matrix $\mathcal{M}$ is symmetric positive definite, and $\mathcal{S}$ is symmetric positive semidefinite. The matrix $X\Lambda^s X^{-1}$ in (2.9) is the s -th power of the matrix $A = \mathcal{M}^{-1}\mathcal{S}$, and consequently:*

- (i) *in the case of a homogeneous Dirichlet boundary condition, $\mathcal{S}$ is positive definite and $A := \mathcal{M}^{-1}\mathcal{S}$ has N_h real positive eigenvalues;*
- (ii) *in the case of a homogeneous Neumann boundary condition, $\ker \mathcal{S} = \text{span}\{(1, \dots, 1)^T\}$ and $A := \mathcal{M}^{-1}\mathcal{S}$ has the simple eigenvalue 0, with eigenvector $(1, \dots, 1)^T$, together with $N_h - 1$ real positive eigenvalues.*

Proof. The symmetry of the matrices $\mathcal{S}$ and $\mathcal{M}$ is obvious. That the matrix $\mathcal{S}$ is positive semidefinite is also easy to prove: suppose that $\xi \in \mathbb{R}^{N_h} \setminus \{0\}$ and let $v(x) := \sum_{i \in \mathcal{J}_h} \xi_i \phi_i(x)$ for $x \in \bar{\Omega}$. Then, $\xi^T \mathcal{S} \xi = \|\nabla v\|_{L^2(\Omega)}^2 \geq 0$. Thanks to the classical Poincaré inequality in $H_0^1(\Omega)$ in the case of $V_h \subset H_0^1(\Omega)$, there exists a positive constant $C = C(\Omega, d)$ such that $\|\nabla v\|_{L^2(\Omega)}^2 \geq C\|v\|_{L^2(\Omega)}^2 > 0$, because $\xi \neq 0$ and the functions $\{\phi_i\}_i$ are linearly independent. Hence $\mathcal{S}$ is positive definite in the case of a homogeneous Dirichlet boundary condition. The positive definiteness of the matrix $\mathcal{M}$ follows even more directly: $\xi^T \mathcal{M} \xi = \|v\|_{L^2(\Omega)}^2 > 0$, again because $\xi \neq 0$ and the functions $\{\phi_i\}_{i \in \mathcal{J}_h}$ are linearly independent. In particular, $\mathcal{M}$ is an invertible matrix and $\mathcal{S}$ is invertible on $(\text{span}\{(1, \dots, 1)^T\})^\perp$.

Let us restate (2.5) by expressing the eigenfunction φ_h in terms of the nodal basis using the numbering of eigenvalues and eigenfunctions of the Dirichlet case without loss of generality (a parallel expression with indices shifted down by one would hold for the Neumann case): $\varphi_h = \sum_{i \in \mathcal{J}_h} (\varphi_h)_i \phi_i$, with $(\varphi_h)_i \in \mathbb{R}$. The eigenproblem reduces to the equality $\sum_{i \in \mathcal{J}_h} (\nabla \phi_i, \nabla \phi_j) (\varphi_h)_i = \lambda^h \sum_{i \in \mathcal{J}_h} (\phi_i, \phi_j) (\varphi_h)_i$, which can be rewritten in matrix form as the generalized algebraic eigenvalue problem

$$\mathcal{S}\Phi = \lambda^h \mathcal{M}\Phi, \quad (2.10)$$

where $\Phi = ((\varphi_h)_1, \dots, (\varphi_h)_{N_h})^T \in \mathbb{R}^{N_h}$. Equation (2.10) implies that λ_j^h is an eigenvalue of the matrix $\mathcal{M}^{-1}\mathcal{S}$ with associated eigenvector Φ_j . Therefore, the matrix X introduced prior to equation (2.9) has the form $X = [\Phi_1, \dots, \Phi_{N_h}] \in \mathbb{R}^{N_h \times N_h}$. Consequently, the matrix $X\Lambda^s X^{-1}$ is the s -th power of $A = \mathcal{M}^{-1}\mathcal{S}$. Finally, in the case of Dirichlet boundary conditions, because

the symmetric matrices $\mathcal{S} \in \mathbb{R}^{\mathcal{N}_h \times \mathcal{N}_h}$ and $\mathcal{M} \in \mathbb{R}^{\mathcal{N}_h \times \mathcal{N}_h}$ are positive definite, it follows that the $\mathcal{N}_h$ eigenvalues λ^h of the matrix A are real and positive. In the case of Neumann boundary conditions one eigenvalue is 0, corresponding to the kernel of $\mathcal{S}$, the remaining $\mathcal{N}_h - 1$ are positive. $\square$

Remark 2.2. From a practical perspective, at the level of the implementation, to ensure solvability of the system (2.9) in the case of a Neumann boundary condition, where the kernel of the matrix A is nontrivial, we always need either that the vector F belongs to the $(\text{span}\{(1, \dots, 1)^T\})^\perp$ or that F is projected into it by choosing $F - \frac{1}{\mathcal{N}_h} (\sum_i F_i) (1, \dots, 1)^T$.

2.1 Rational approximation and fractional powers of a matrix

According to Lemma 2.1 our finite element approximation of the fractional Poisson equation involves the computation of the fractional power of a matrix A . The use of this method, particularly in two or higher dimensions, tends to be avoided in practice because the computational cost to obtain an approximation of the power of a matrix is usually high for large matrices. As we mentioned at the beginning of the chapter we would require a priori knowledge of the spectral properties of the matrix itself: as the dimension of the matrix increases, one needs to compute an increasing number of eigenvalues and eigenvectors to improve the accuracy of the method, which is, for very large matrices, practically infeasible. In addition to this difficulty, there are also difficulties of storage because the matrix A is dense, since it corresponds to the discretization of a nonlocal operator.

The algorithm that we shall describe has been proposed precisely to overcome these difficulties and hence to develop a computationally efficient procedure to approximate fractional powers of a matrix A . More precisely, our focus is the approximation of the matrix A^{-s} , to directly solve the linear system (2.9). The fundamental component of the algorithm is the use of rational approximations.

Over the past decades, many algorithms were developed for the computation of rational approximations of functions and their application to problems in numerical linear algebra, [53, 120, 106], and the recent work [176] has continued along this direction. In our work we intend to use the *minimax algorithm* developed in [106]. We show that this algorithm is particularly helpful in the present context, as it provides the high precision predicted by rational approximation theory while maintaining excellent computational efficiency. The minimax strategy is based on the AAA algorithm for rational approximations [145] and a classical Remez algorithm. Exploring the use of alternative rational approximation algorithms (e.g. BURA [120]) for the type of evolution problem considered here constitutes an interesting alternative. As a matter of fact, we refer to [119] for one example of a comparative analysis of BURA with other numerical methods, including AAA, for a one-dimensional elliptic fractional problem, $(-d^2/dx^2)^s u = 1$ on

$\Omega = (-1, 1)$, discretized with piecewise linear finite elements: the comparison, done with respect to accuracy and degree of rational approximation, already showed that, even if the errors of AAA and BURA have a similar behaviour, the error of the AAA method is always smaller than the error of BURA method (see [119, Remark 6.1]). Moreover [119, Section 7] highlights challenges beyond the scalar elliptic case, with a discussion of time dependent space-fractional diffusion problems; this further motivates our application of minimax to evolutionary nonlinear problems involving the spectral fractional Laplacian. We also mention [52] for some recent work in this direction, for a different PDE model unrelated to the fractional Laplacian.

The minimax algorithm was developed to compute the best rational approximation of a given function in one variable, on a given interval, through adaptive barycentric representations. We briefly outline the method, and we refer to [106] for further details.

Let

$$\mathcal{R}_{m,n} := \left\{ \frac{p}{q} : p \in \mathbb{P}_m[x], \quad q \in \mathbb{P}_n[x] \right\} \quad (2.11)$$

denote the set of rational functions of type (m, n) , where $\mathbb{P}_n[x]$ denotes the set of all polynomials in x of degree at most n . Given a continuous real-valued function g defined on a closed interval $[a, b] \subset \mathbb{R}$, the algorithm computes an approximation of the solution to the problem

$$\inf_{r \in \mathcal{R}_{m,n}} \|g - r\|_{\infty, [a,b]}, \quad (2.12)$$

where $\|\cdot\|_{\infty, [a,b]}$ denotes the maximum norm over $[a, b]$, i.e. $\|g - r\|_{\infty, [a,b]} = \max_{x \in [a,b]} |g(x) - r(x)|$. We denote by $r_{m,n}^*$ the solution of the problem, called the *best rational approximation*.

For the sake of simplicity, we shall restrict our attention to the case $m = n$. Working in this setting will enable us in Section 2.1.1 to make direct use of a sharp estimate due to a renowned result by Stahl [165], stated in Remark 2.5. We shall seek the best rational approximation r of type (n, n) to g in its partial fraction representation, i.e. as

$$r(x) = R_0 + \frac{R_1}{x - t_1} + \cdots + \frac{R_n}{x - t_n},$$

where $t_1, \dots, t_n$ are the poles of r , and the numbers $R_0, R_1, \dots, R_n$ are referred to as the residues of r . It is known (cf. [158, Lemma 2.1]) that the poles of the best rational approximation are real and negative. The minimax algorithm from [106] provides the user with both the residues and poles of the best rational approximation.

The method is then suitable for the approximation of the matrix function $M \in \mathbb{R}^{N \times N} \mapsto g(M) \in \mathbb{R}^{N \times N}$ using the corresponding expression

$$r(M) = R_0 I + R_1 (M - t_1 I)^{-1} + \cdots + R_n (M - t_n I)^{-1}. \quad (2.13)$$

We will approximate here $g(x) = x^{-s}$ by a rational function $r \in \mathcal{R}_{n,n}$, which will then provide the desired matrix approximation to the fractional power A^{-s} of the matrix A under consideration.

Remark 2.3 (Efficiency: computational cost). Once we have the residues and poles of the rational approximation r , and thereby the rational approximation $r(A)$ of the matrix A^{-s} , it is then straightforward to compute an approximation to the vector $U = g(A)F$ in (2.9) as

$$r(A)F = R_0F + R_1(A - t_1I)^{-1}F + \cdots + R_n(A - t_nI)^{-1}F. \quad (2.14)$$

The terms $T_i := R_i(A - t_iI)^{-1}F$ appearing on the right-hand side of (2.14) can be efficiently computed by solving systems of linear algebraic equations of the form $(A - t_iI)T_i = R_iF$, $i = 1, \dots, n$. In the present context, $A = \mathcal{M}^{-1}\mathcal{S}$ (cf. Lemma 2.1).

From a computational perspective, we observe that applying mass lumping to the symmetric positive definite mass matrix $\mathcal{M}$, thus replacing $\mathcal{M}$ with a positive definite diagonal matrix $\hat{\mathcal{M}}$, results in a matrix $\hat{A} = \hat{\mathcal{M}}^{-1}\mathcal{S}$, which has the same sparsity structure as the stiffness matrix $\mathcal{S}$. As a result, the matrices $(\hat{A} - t_iI)$ retain the sparsity structure of $\mathcal{S}$, and this enhances the efficiency of solving the associated linear systems when using a finite element nodal basis.

The degree n of the rational approximation r is typically a small number (common choices are $n = 11, 12, 13$) to ensure sufficient accuracy. Thus, once the minimax algorithm has provided us with the residues and poles, the overall complexity of computing $r(A)F$ is $\mathcal{O}(n\mathcal{C}(N))$, where $\mathcal{C}(N)$ is the cost of solving the linear systems specified above. This fact is particularly well-suited for nonlinear and time dependent problems that involve the fractional Laplacian and where a solution $r(A)F$ has to be computed at each time step of the discrete-in-time approximation. In addition, problems of storage when N_h increases (encountered for example in [14] where a full matrix approximating fractional diffusion had to be stored) are avoided, since the only data to be saved and read are n residues and poles and a sparse matrix. To appreciate this advantage we observe that for $N_h = 2^{14}$, a dense $N_h \times N_h$ matrix would require 2 gigabytes of RAM. For $N_h = 2^{16}$, the size would be 16 gigabytes, or 128 gigabytes for $N_h = 2^{18}$.

Remark 2.4 (Efficiency: knowledge of the spectrum). We note that, thanks to the nature of the minimax algorithm developed in [106], to compute the best rational approximation to the function x^{-s} , our method does not require the spectrum of the discrete Laplacian $-\Delta_h$. The algorithm only needs the endpoints x_{min}, x_{max} of the interval $[x_{min}, x_{max}]$ on which the user aims to build the approximation. This is of significant benefit in computing $r(A)$, since we only require estimates of the smallest and largest eigenvalues of the matrix A , and these can be easily calculated using standard algorithms from numerical linear algebra. We remark that this advantage is also present in the previous work [117], which computes fractional powers and other functions of matrices using a different approach, based on contour integrals and conformal maps. However the performance of the methods described in [117], even though suitable for general functions of matrices, do not outperform best rational approximations for fractional powers, particularly when $x_{max} \gg x_{min}$, as discussed in [117, Section 5] for the specific case $s = 1/2$.

Remark 2.5 (Error estimate). It was proved by Stahl [165] that the error of best rational approximation exhibits root-exponential decay with respect to the degree of the rational approximation. More precisely, letting $r_{n,n}^*(x)$ denote the best rational approximation to x^s , $s > 0$, with degree $n \in \mathbb{N}$, Stahl proved that, defining $E_{n,n}(x^s, [0, 1]) := \|x^s - r_{n,n}^*(x)\|_{\infty, [0, 1]} = \inf_{r \in \mathcal{R}_{n,n}} \|x^s - r(x)\|_{\infty, [0, 1]}$, one has that

$$\lim_{n \rightarrow \infty} e^{2\pi\sqrt{sn}} E_{n,n}(x^s, [0, 1]) = 4^{1+s} |\sin(\pi s)|. \quad (2.15)$$

As a consequence, there is a constant $C_s > 0$ such that

$$E_{n,n}(x^s, [0, 1]) \leq C_s e^{-2\pi\sqrt{sn}}. \quad (2.16)$$

2.1.1 Error analysis

We now provide an error estimate in $L^2(\Omega)$ norm for the numerical method that we have presented, combining the existing results on FEM approximation of the fractional Laplacian and the ones on rational approximations, while testing numerically the errors and validating the estimates for several values of the fractional order s , both in one and two dimensions.

Let us consider the error $\|u^* - u_h\|_{L^2(\Omega)}$ in the $L^2(\Omega)$ norm, where u^* is the exact solution to the fractional Poisson equation

$$(-\Delta_{\mathcal{B}})^s u^* = f \quad \text{in } \Omega$$

subject to a homogeneous Dirichlet or homogeneous Neumann boundary condition on $\partial\Omega$, with $\int_{\Omega} f \, dx = 0$ in case of a Neumann boundary condition, and let u_h be the numerical solution obtained by our method, based on combining the finite element approximation of u^* with a rational approximation $r^*(A)$ of A^{-s} where $A := \mathcal{M}^{-1}\mathcal{S}$, i.e.

$$u_h := \mathcal{I}_h(r^*(\mathcal{M}^{-1}\mathcal{S})F) = \mathcal{I}_h(r^*(A)F), \quad (2.17)$$

where $\mathcal{I}_h$ is the interpolation operator defined in (2.3) and F is the vector defined in (2.9). Since $r^*(A)$ is an approximation of the inverse power matrix A^{-s} , we split the total error $u^* - u_h$ into two parts, given the two stages of our approximation to u^* ; thus,

$$\begin{aligned} \|u^* - u_h\|_{L^2(\Omega)} &\leq \|u^* - \mathcal{I}_h(A^{-s}F)\|_{L^2(\Omega)} + \|\mathcal{I}_h(A^{-s}F) - \mathcal{I}_h(r^*(A)F)\|_{L^2(\Omega)} \\ &:= E_{\text{FEM}} + E_{\text{MIM}}. \end{aligned} \quad (2.18)$$

The first term E_{FEM} exhibits the order of convergence in the limit of $h \rightarrow 0_+$ of the finite element approximation $(-\Delta_h)^s$ to the fractional Laplacian, and is governed by [43, Theorem 4.3] and subsequent generalizations (see [44, Theorem 6.2] and [39]).

Considering the second term E_{MIM} , we propose an adaptation of the error estimate of [120] to our specific case. Since $\mathcal{I}_h(A^{-s}F) - \mathcal{I}_h(r^*(A)F) \in V_h$, by norm-equivalence in finite-dimensional

normed linear spaces, we can pass from the $L^2(\Omega)$ norm to the Euclidean 2-norm $\|\cdot\|_2$, up to a factor $C(h, d)$, depending on the mesh-size h and the dimension d of the computational domain Ω . Therefore, we have

$$\begin{aligned}
E_{\text{MIM}} &\leq C(h, d) \|A^{-s}F - r^*(A)F\|_2 \leq C(h, d) \|A^{-s} - r^*(A)\|_2 \|F\|_2 \\
&\leq C(h, d) \|X\Lambda^{-s}X^{-1} - Xr^*(\Lambda)X^{-1}\|_2 \|F\|_2 \\
&\leq C(h, d) \|X\|_2 \|X^{-1}\|_2 \|\Lambda^{-s} - r^*(\Lambda)\|_2 \|F\|_2 \\
&= C(h, d) \kappa_2(X) \left(\max_{1 \leq i \leq N_h} |(\lambda_i^h)^{-s} - r^*((\lambda_i^h))| \right) \|F\|_2,
\end{aligned} \tag{2.19}$$

where $\kappa_2(X) := \|X\|_2 \|X^{-1}\|_2$ is the condition number of the matrix X , and $\{\lambda_k^h\}_{k=1}^{N_h}$ are the eigenvalues of the matrix $A = \mathcal{M}^{-1}\mathcal{S}$ (cf. Lemma 2.1); when applied to a matrix, $\|\cdot\|_2$ signifies the matrix 2-norm. Since the discrete spectral fractional Laplacian $-\Delta_h$ is a positive self-adjoint operator, we have $0 < \lambda_1^h \leq \lambda_2^h \leq \dots \leq \lambda_{N_h}^h$, and $N_h \rightarrow \infty$ as $h \rightarrow 0$. It is known that $\lambda_1^h \rightarrow \lambda_1$ as $h \rightarrow 0$. For a quasi-uniform triangulation it is easy to prove that the constant $C(h, d) \sim h^{d/2}$.

We shall now use the estimate (2.15) from Remark 2.5. By rescaling the computational domain Ω , if necessary, one can assume without loss of generality that $\lambda_1 > 1$ and $\lambda_1^h > 1$ for all $h > 0$; hence,

$$\begin{aligned}
E_{\text{MIM}} &\leq C(h, d) \kappa_2(X) \|x^{-s} - r_{n,n}^*(x)\|_{\infty, [1, \infty)} \|F\|_2 \\
&= C(h, d) \kappa_2(X) \inf_{r \in \mathcal{R}_{n,n}} \|x^{-s} - r(x)\|_{\infty, [1, \infty)} \|F\|_2.
\end{aligned}$$

By using the change of variable $y = x^{-1}$ it then follows that

$$E_{\text{MIM}} \leq C(h, d) \kappa_2(X) \inf_{r \in \mathcal{R}_{n,n}} \|y^s - r(y^{-1})\|_{\infty, (0, 1]} \|F\|_2 \tag{2.20}$$

$$\begin{aligned}
&= C(h, d) \kappa_2(X) \inf_{r \in \mathcal{R}_{n,n}} \|y^s - \hat{r}(y)\|_{\infty, (0, 1]} \|F\|_2 \\
&= C(h, d) \kappa_2(X) \inf_{r \in \mathcal{R}_{n,n}} \|y^s - r(y)\|_{\infty, (0, 1]} \|F\|_2,
\end{aligned} \tag{2.21}$$

where in the last equality we have used the fact that $\hat{r}(y) := r(y^{-1})$ is still a rational function of degree $m = n$ if r is a rational function of degree $m = n$; indeed, thanks to the definition (2.11), we have $\{\hat{r}(y) : r \in \mathcal{R}_{n,n}\} = \mathcal{R}_{n,n}$. Extending by continuity from $(0, 1]$ to $[0, 1]$ and using (2.16) we finally have that

$$E_{\text{MIM}} \leq C_s C(h, d) \kappa_2(X) e^{-2\pi\sqrt{sn}}, \tag{2.22}$$

for a positive constant C_s depending only on s .

This result, together with the bound E_{FEM} on the error committed in the finite element approximation, gives us control of the $L^2(\Omega)$ norm error appearing on the left-hand side of the inequality (2.18). The user can thereby prescribe the degree n of the rational approximation and the mesh size h to achieve the desired overall accuracy. Once the mesh size h is fixed, thanks to the root-exponential decay with respect to n of the final factor on the right-hand side of the

Table 2.1: The fractional Poisson equation (2.1) in Ω with homogeneous Dirichlet boundary condition; study of the convergence order as a function of the mesh size h for $f \equiv 1$. We compare the observed order of convergence with the predicted order of convergence, as stated in [43, Theorem 4.3 and Remark 4.1]. Here, by *order of convergence* we mean the exponent $2r$ in $C_h h^{2r}$, ignoring the presence of the factor $\log(1/h)$ in C_h when $s \leq 3/4$; cf. (2.23).

	$s < \frac{3}{4}$						$s > \frac{3}{4}$	
	0.02	0.05	0.1	0.25	0.5	0.67	0.83	0.9
1D $\Omega = (0, 1)$								
observed	0.5400	0.6000	0.6600	1.0003	1.5033	1.7922	1.9227	2.0664
2D $\Omega = (0, 1)^2$								
observed	0.5214	0.5816	0.6821	0.9843	1.4912	1.7988	1.9598	1.9804
predicted	0.54	0.6	0.7	1.0	1.5	1.83	2.0	2.0

inequality (2.22), it is possible to choose the optimal degree n for the rational approximation to obtain the same level of accuracy in E_{MIM} as in E_{FEM} and compensate for the presence of the factor $C(h, d)$.

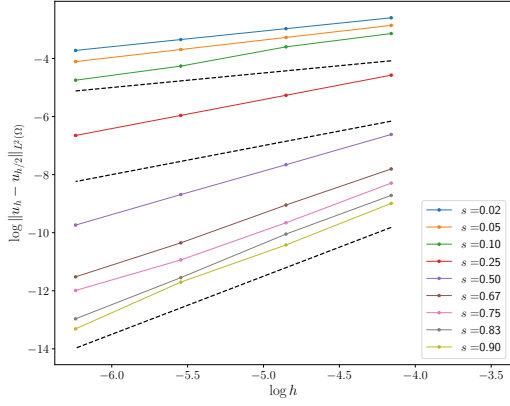
We now test numerically the convergence orders of the two sources of error in (2.18), E_{FEM} and E_{MIM} , with our convergence results reported in Figures 2.1a, 2.1b, 2.3. In particular, on one hand in Figures 2.1a and 2.1b we assess in one and two space dimensions, respectively, the order of convergence of our method as $h \rightarrow 0$, governed by the term E_{FEM} , on the other hand in Figure 2.3 we validate our estimate of the error E_{MIM} .

The derivation of a bound on the error E_{FEM} has been studied in recent years, and its rate of convergence in the limit of $h \rightarrow 0$ is known (see [43, Theorem 4.3 and Remark 4.1]). In order to validate these known results with our method, we use a specific case: for $f \in \mathbb{H}^{\frac{1}{2}-\epsilon}(\Omega)$ with arbitrarily small $\epsilon > 0$ the authors of [43] showed that the FEM error E_{FEM} is bounded above by $C_h h^{2r}$, where

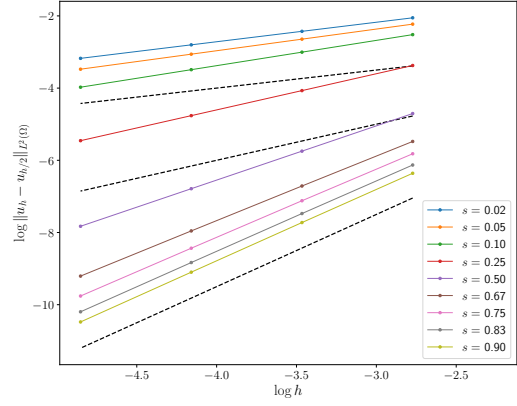
$$C_h = \begin{cases} C & \text{if } s > \frac{3}{4}, \\ C \log(1/h) & \text{otherwise,} \end{cases} \quad r = \begin{cases} 1 & \text{if } s > \frac{3}{4}, \\ s + \frac{1}{4} & \text{otherwise;} \end{cases} \quad (2.23)$$

this is in fact a simple application of the result that we stated in Chapter 1, Proposition 1.13 that we reported from [43]. The values of the slopes of the curves in the convergence graphs in Figures 2.1a, 2.1b are reported in Table 2.1; we can appreciate how the observed order of convergence in h matches the predicted one that is stated in (2.23) in both the one- and two-dimensional case for the different values of s .

In Figure 2.3 we validate our estimate of the error E_{MIM} associated with the rational approximation and report the order of convergence with respect to the degree n of the best rational approximation (2.12). We observe that, with the mesh size $h > 0$ fixed, the order of convergence in the limit of $n \rightarrow \infty$ is actually exponential rather than root-exponential as predicted by (2.22). This discrepancy is due to the difference in the domains over which the errors are

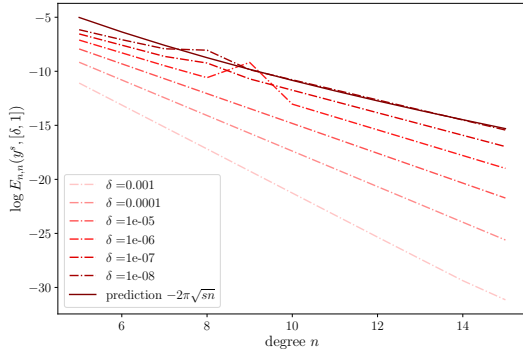


(a) One-dimensional case $\Omega = (0, 1)$. Mesh sizes $h = 1/2^k$ with $5 \leq k \leq 9$ were used.

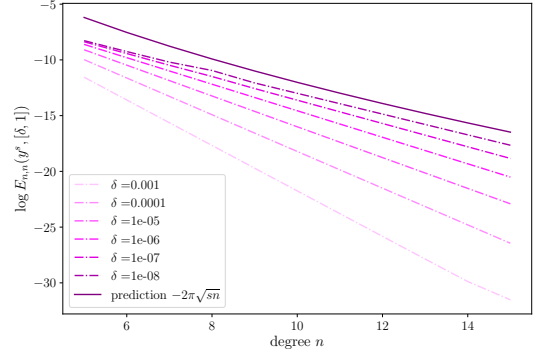


(b) Two-dimensional case $\Omega = (0, 1)^2$. Mesh sizes $h = 1/2^k$ with $3 \leq k \leq 7$ were used.

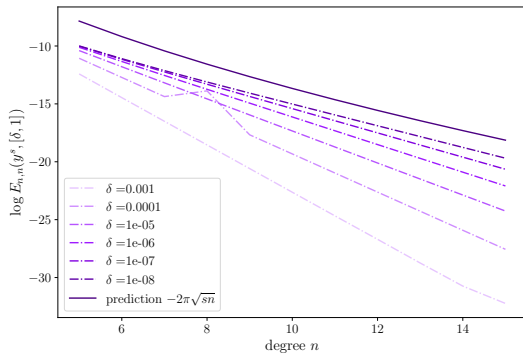
Figure 2.1: The fractional Poisson equation (2.1) in Ω with homogeneous Dirichlet boundary condition; study of the convergence order as a function of the mesh size h . We report the convergence of the scheme for $f \equiv 1$. The black reference lines have slope, respectively, 2, 1.5, and 1.



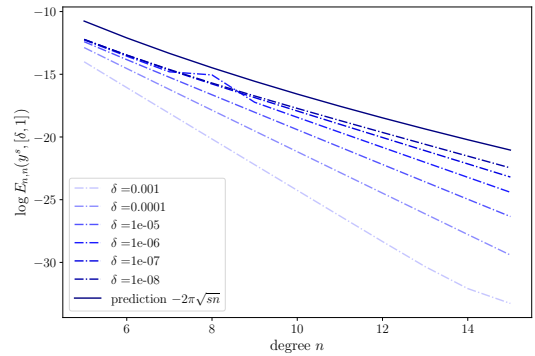
(a) $s = 0.2$



(b) $s = 0.5$



(c) $s = 0.7$



(d) $s = 0.9$

Figure 2.2: Rational approximation of $f(y) = y^s$ computed through the minimax algorithm on intervals $[\delta, 1]$ for $\delta > 0$. Computation of the error $E_{n,n}(y^s, [\delta, 1]) := \|y^s - r_{n,n}^*(y)\|_{\infty, [\delta, 1]} = \inf_{r \in \mathcal{R}_{n,n}} \|y^s - r(y)\|_{\infty, [\delta, 1]}$ and comparison with the prediction (2.15) for $E_{n,n}(y^s, [0, 1])$.

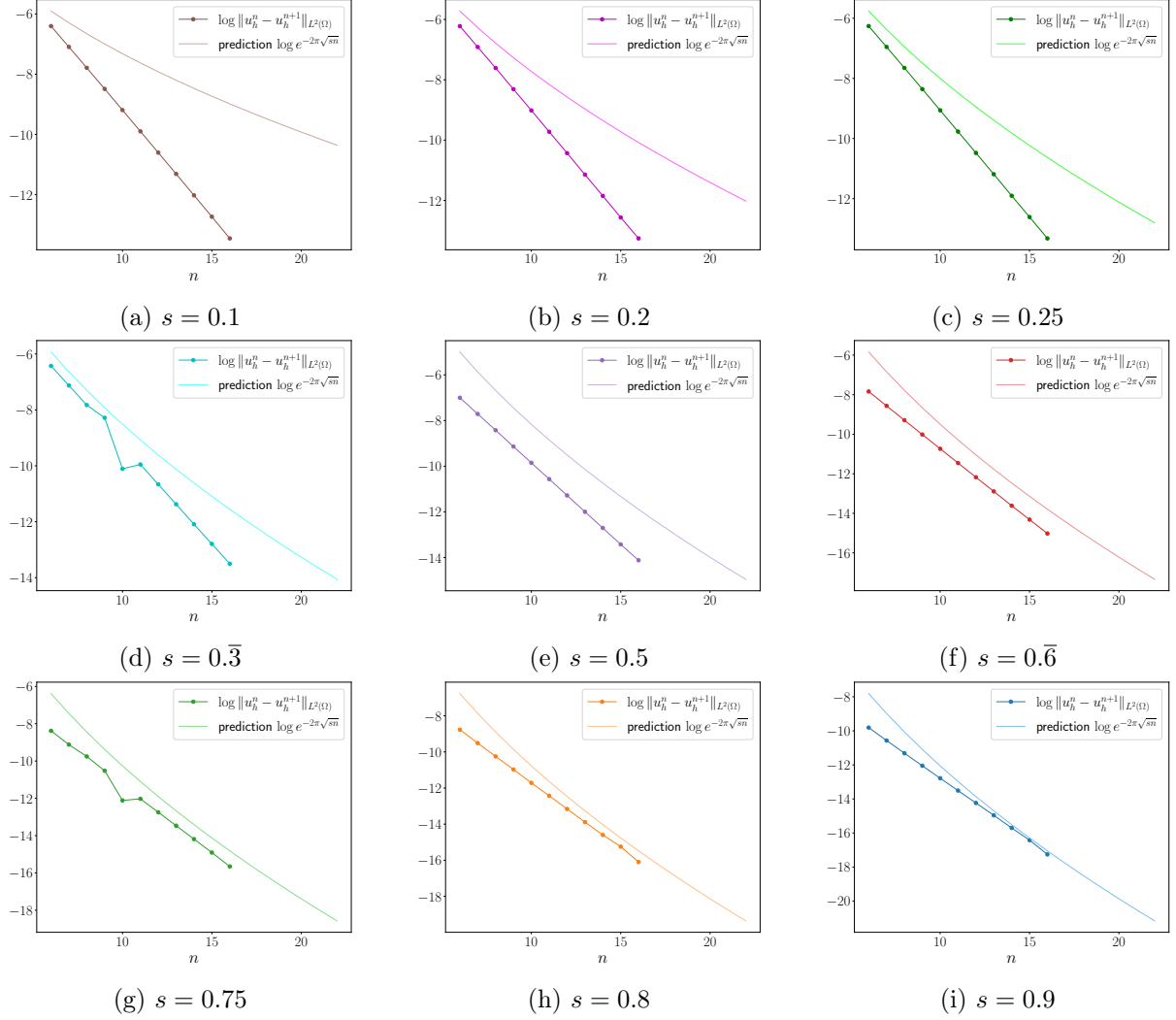


Figure 2.3: The fractional Poisson equation: the observed exponential convergence of the best rational approximation (2.12), used in (2.14). The computation of the function u_h^n defined in (2.17) was performed for different fractional orders to assess the $L^2(\Omega)$ norm of the difference between u_h^n and u_h^{n+1} as a function of the degree n of rational approximation, in comparison with the theoretical prediction (2.22). Each solution was computed on $\Omega = (0, 1)^2$ with $f(x, y) = \sin(\pi x) \sin(\pi y)$, and with a mesh of $2^8 \times 2^8$ equally spaced mesh points.

evaluated. Specifically, the estimate (2.22) was based on bounding the sup-norm over the whole interval $y \in [0, 1]$, while, as can be seen from (2.19), our bound on the actual error E_{MIM} only involves the sup-norm over the subinterval $y \in [(\lambda_{N_h}^h)^{-1}, (\lambda_1^h)^{-1}] \subset [0, 1]$; crucially, the interval $[(\lambda_{N_h}^h)^{-1}, (\lambda_1^h)^{-1}]$ excludes the ‘singular point’ $y = 0$, at which the function $y \in [0, 1] \mapsto y^s$ has unbounded derivatives for all $s \in (0, 1)$. This renders the minimax approximation a very accurate computational technique over the subinterval $[(\lambda_{N_h}^h)^{-1}, (\lambda_1^h)^{-1}]$ and substantiates the common choice of relatively low values of the degree n of rational approximation, $n = 11, 12, 13$ being typical choices in practice. In Figure 2.2 we numerically validate our reasoning as to why exponential rather than slower root-exponential convergence is observed in the results reported in Figure 2.3. We compute rational approximations of the function $f(y) = y^s$ for different fractional orders $s \in (0, 1)$ on intervals of the form $[\delta, 1]$ with $\delta > 0$. As we can see in Figure 2.2, for all fractional orders, as δ decreases toward zero, the convergence in n becomes slower, reaching the root-exponential convergence predicted by the estimate (2.15) for the interval $[0, 1]$.

2.2 Numerical experiments on related evolution problems

We now present the results of applying the method described in Section 2.1 for the finite element approximation of the spectral fractional Laplacian to the evolutionary PDEs of our interest. We focus on the fractional porous medium equation that we have discussed in Chapter 1 and a related model, that is the fractional Keller–Segel equation. The reason for doing this is because the two equations are closely related as they both feature a potential term, which is the solution to a fractional Poisson equation. However, in the fractional porous medium equation, the potential is repulsive, promoting the dispersion of the density in space, whereas in the Keller–Segel model, the potential is attractive, leading to an aggregation effect. While for the fractional porous medium we can give a mathematical foundation to the simulations with the convergent scheme that we have developed in Chapter 1, for the fractional Keller–Segel equation the development of a convergent scheme is more challenging because the solution can develop singularities in finite time. Both phenomena are however of significant interest and have numerous applications. From a purely scientific computing perspective, the algorithm allows us to simulate the different equations in two dimensions for different fractional orders. On the one hand, the results will allow us to validate certain properties of our scheme for the fractional porous medium equation; on the other hand, they will provide a numerical exploration of the fractional Keller–Segel model. For the latter we will present a theoretical result regarding the blow-up of the solution.

From an implementation perspective, the schemes used for the computations in the following sections consist of a FE weak formulation paired with a Euler implicit time stepping for the time discretisation. We take no cut-offs, corresponding to $\delta = 0$ and $L = +\infty$ in (1.13). Denoting by ρ_h^n the approximate solution at the n -th time step, for the nonlinear terms involving the potential, $\rho \nabla c$, we keep a scalar nonlinearity at the level of implementation, using $\rho_h^n I \nabla c_h^n$. The

implementation uses Firedrake [118], with Gmsh [110] for mesh generation, to assemble the stiffness and mass matrices for the standard Laplacian that are used in the rational approximation of the spectral fractional Laplacian. At each time step the resulting nonlinear system is solved with `NonlinearVariationalProblem` and `NonlinearVariationalSolver`.

2.2.1 The fractional porous medium equation

Let us consider the parabolic regularisation for the fractional porous medium equation (1.2), where we control the parabolic regularisation through a parameter $\mu > 0$, namely

$$\frac{\partial \rho}{\partial t} = \mu \Delta \rho - \nabla \cdot (\rho \nabla c), \quad -(-\Delta_N)^s c = \rho^*, \quad 0 < s < 1. \quad (2.24)$$

Before computationally exploring the behaviour of the model, we shall validate our finite element scheme.

We recall that for $s \rightarrow 0$ the equation tends to a standard porous medium equation with Fickian diffusion.

$$\frac{\partial \rho}{\partial t} = \mu \Delta \rho + \nabla \cdot (\rho \nabla \rho). \quad (2.25)$$

Therefore, in the first place, we shall validate the method by studying the asymptotic decay towards the equilibrium solution of the following Fokker–Planck equation:

$$\frac{\partial \rho}{\partial t} = \mu \Delta \rho + \nabla \cdot (\rho \nabla \rho) + \nabla \cdot (x \rho) = \nabla \cdot \left(\rho \nabla \left(F(\rho) + \frac{|x|^2}{2} \right) \right). \quad (2.26)$$

An explicit steady-state solution to this equation can be computed on the whole of $\mathbb{R}^d$ as

$$\rho^{\text{Std}}(x) = F^{-1} \left(-\frac{|x|^2}{2} + C \right), \quad \text{where } F(\psi) = \mu \log(\psi) + \psi \quad (2.27)$$

and C is a constant whose value is fixed by the mass of the positive initial datum. Denoting by ρ_h for simplicity the approximate solution that we compute using our finite element approximation, in Figure 2.4 we report the $L^2(\Omega)$ norm of the difference between ρ^{Std} and ρ_h . We observe convergence up to the precision provided by the computational mesh.

Now, let us consider the fractional porous medium equation without the Fickian diffusion term, that is, for $\mu = 0$ in (2.24):

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \nabla c), \quad -(-\Delta_N)^s c = \rho^*, \quad 0 < s < 1,$$

for which there exists a family of self-similar profiles on the whole of $\mathbb{R}^d$, cf. [29, 30]. In order to further validate our method, we consider the solution of the corresponding Fokker–Planck equation

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \nabla c) + \nu \nabla \cdot (x \rho), \quad -(-\Delta_N)^s c = \rho^*, \quad 0 < s < 1, \quad \nu = \frac{1}{d+2-2s} \quad (2.28)$$

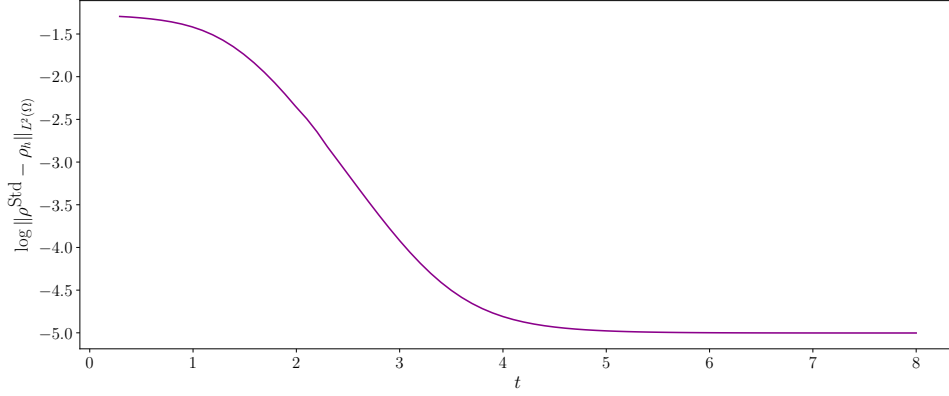


Figure 2.4: The porous medium equation (2.26) in self-similar variables; convergence to the steady state (2.27) for $s = 2^{-10}$. The computational domain is $\Omega = B_R(0)$, $R = 10$, $\mu = 1$, a mesh of 37267 uniformly spaced mesh points was used with $\Delta t = 0.01$.

that admits a steady state on the whole of $\mathbb{R}^d$, given by

$$\Phi_s(y) = k_{s,d}(1 - |y|^2)_+^{1-s}, \quad \text{with } k_{s,d} = \frac{d\Gamma(d/2)}{(d + 2(1-s))2^{2(1-s)}\Gamma(2-s)\Gamma(d/2 + 1-s)}. \quad (2.29)$$

We test our method by applying it to the equation

$$\frac{\partial \rho}{\partial t} = \mu \Delta \rho - \nabla \cdot (\rho \nabla c) + \nu \nabla \cdot (x \rho), \quad -(-\Delta_N)^s c = \rho^*, \quad 0 < s < 1, \quad (2.30)$$

for very small values of μ and compare the numerically computed steady states that we compute with (2.29). In doing this, however, it needs to be borne in mind that (2.29) does not belong to $H^1(\Omega)$, but only to $H^{1-s}(\Omega)$ with $s \in [0, 1)$. This is reflected in our numerical results by the fact that, for a fixed mesh size, as μ becomes smaller, our numerical solution develops oscillations in a small neighbourhood of the unit circle $\{y \in \mathbb{R}^2, |y| = 1\}$, where the H^1 regularity of the solution is lost. This is expected behaviour, since we are using a finite element method that relies on the presence of the parabolic regularisation term $\mu \Delta \rho$. In the experiments reported in Figure 2.5, 2.6, 2.7, 2.8 the initial datum $\rho_0 \geq 0$ is chosen proportional to the constant function on Ω , where the constant of proportionality is set such that $\int_{\Omega} \Phi_s(y) dy = \int_{\Omega} \rho_0(y) dy$. In Figure 2.5 we report the results for selected values of μ . While we observe local oscillations developing as μ decreases, we also see that away from the unit circle the profile of the numerical solution approaches the analytical solution profile (2.29). This example also highlights that, since our method is defined for a general finite element discretization, the algorithm admits the use of locally refined computational meshes; indeed, the local oscillations are mitigated by local mesh refinement in the vicinity of the unit circle.

Finally, for a closer inspection of the effect of having a parabolic regularisation, in Figure 2.6 and Figure 2.7 we report the simulations performed for equation (2.30) for a larger range of different values of μ . We can observe the effect of the term $\mu \Delta \rho$, which introduces Brownian

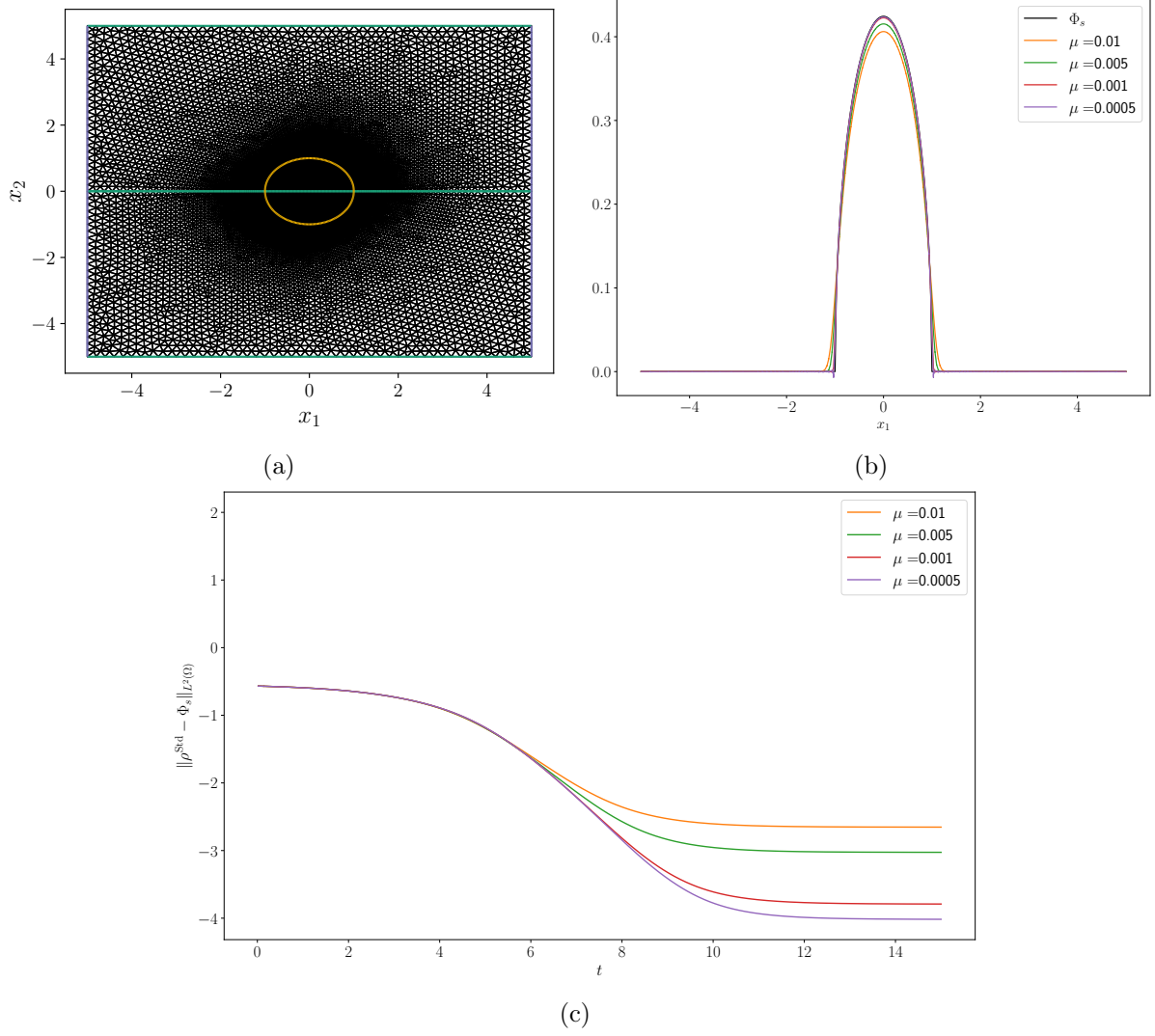


Figure 2.5: The fractional porous medium equation in self-similar variables (2.30); (a) the locally refined mesh on the computational domain Ω ; (b) steady state solution profile for equation (2.30) for different values of μ ; (c) the $L^2(\Omega)$ error between the computed steady state of (2.30) and the analytical steady state Φ_s . The computational domain is $\Omega = (-5, 5)^2$, $\rho_0(x) \propto \frac{1}{|\Omega|}$, a mesh with 13171 mesh points was used, graded towards the centre of the domain, with the time step taken as $\Delta t = 0.01$.

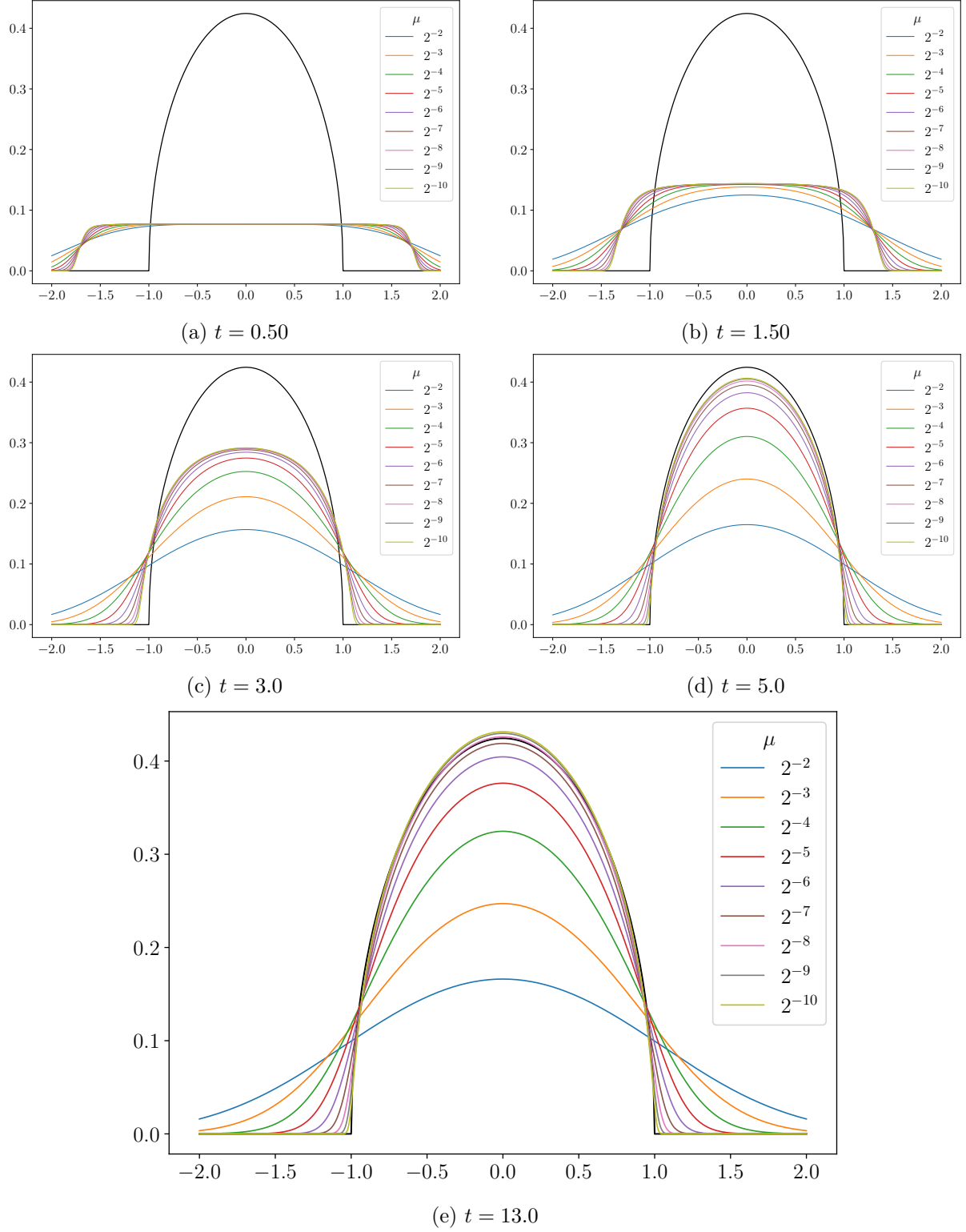


Figure 2.6: Numerical solutions to the fractional porous medium equation in self-similar variables (2.30). The simulations were performed for the fractional order $s = 0.5$ with different values of the parameter $\mu = 2^{-m}$, $m = 2, \dots, 10$, controlling the parabolic regularisation. The computational domain is $\Omega = (-2, 2)^2$, $\rho_0(x) \propto \frac{1}{|\Omega|}$; a uniform triangulation based on $2^9 \times 2^9$ equally spaced nodes was used with $\Delta t = 0.01$. The black reference curve is the cross-section of the function (2.29) at $x_2 = 0$.

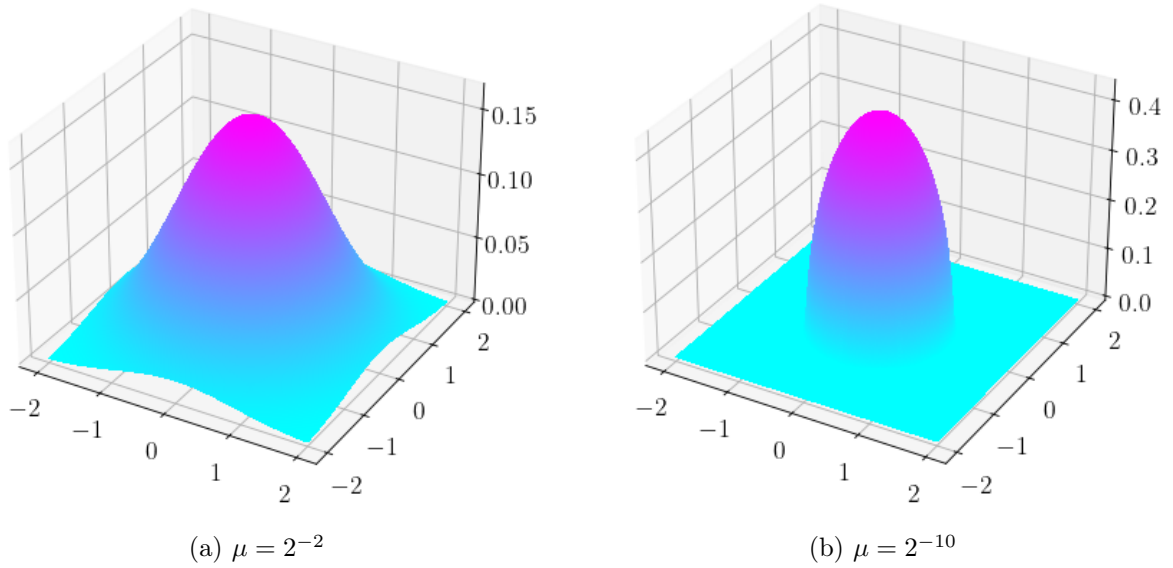


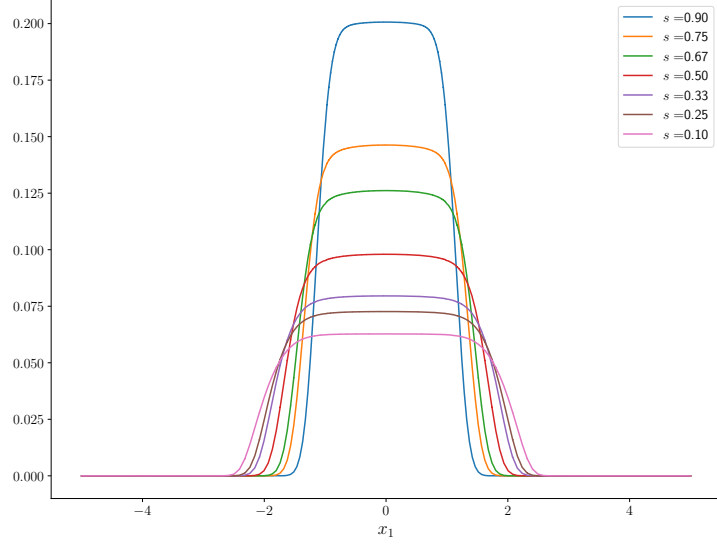
Figure 2.7: Numerical solutions to the fractional porous medium equation in self-similar variables (2.30). The simulations were performed for the fractional order $s = 0.5$ with different values of the parameter $\mu = 2^{-m}$, $m = 2, \dots, 10$, controlling the parabolic regularisation. The computational domain is $\Omega = (-2, 2)^2$, $\rho_0(x) \propto \frac{1}{|\Omega|}$; a uniform triangulation based on $2^9 \times 2^9$ equally spaced nodes was used with $\Delta t = 0.01$.

diffusion of the density, with the numerical solutions still approaching the profile stated in (2.29) as μ decreases.

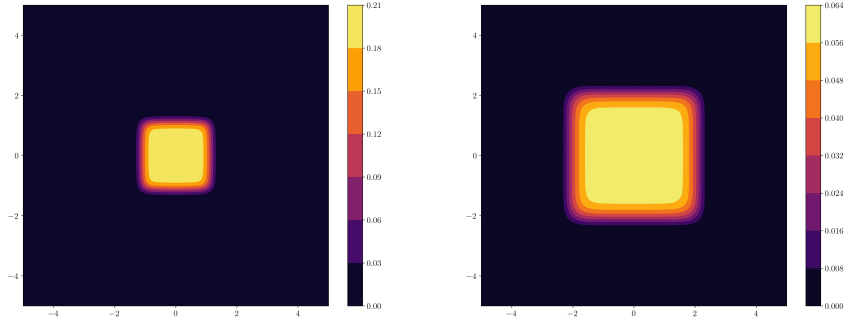
We shall now explore the behaviour of solutions to (2.30) with different values of the fractional order $s \in (0, 1)$. We report the results in Figure 2.8. We observe generic solutions to (2.28) that exhibit the correct qualitative behavior of spreading; see [60, 56]. The solutions are expected to spread according to the self-similar profile stated in equation (2.29) and the 2D simulations reported in Figure 2.8 show that, as $s \rightarrow 0$, the spread becomes more pronounced.

Finally, we check the asymptotics in time of solutions to the fractional porous medium equation stated in Theorem 1.23, where exponential decay of weak solutions of (2.24) to the equilibrium solution is proved, with a rate given by $-2/C_{LS}$, with the logarithmic Sobolev constant C_{LS} satisfying inequality (1.72). We report in Figure 2.9 the rates of convergence to the equilibrium solution for different initial data ρ_0 . Quite interestingly, we see that, for the decay to the equilibrium solution, the lower bound (1.73) for C_{LS} , obtained for $\frac{1}{\lambda_1}$ (λ_1 first positive eigenvalue of the Neumann Laplacian), is observed for the initial data that are the furthest from the equilibrium state: the Gaussian and a blob centred at a corner of the square domain Ω . This numerically suggests that the spectral gap, yielding the Poincaré constant $\frac{1}{\lambda_1}$, could be possibly considered a sharp bound for C_{LS} . We refer the reader to [11] for further discussion on logarithmic Sobolev and Poincaré inequalities for a class of measures on $\mathbb{R}^d$.

It is known that the comparison principle does not hold for the porous medium equation



(a)



(b)

Figure 2.8: Steady state profiles of the fractional porous medium equation (2.30) in self-similar variables with $\mu = 0.01$ for different values of $s \in (0, 1)$. The computational domain is $\Omega = (-5, 5)^2$, $\rho_0(x) \propto \frac{1}{|\Omega|}$; a graded mesh towards the centre of the domain, with 13171 mesh points, was used with the time step taken as $\Delta t = 0.01$. (a): cross-section of the numerical solution at $x_2 = 0$ as a function of x_1 for different values of s ; (b): contour plot for values of $s = 0.9$ (left) and $s = 0.1$ (right).

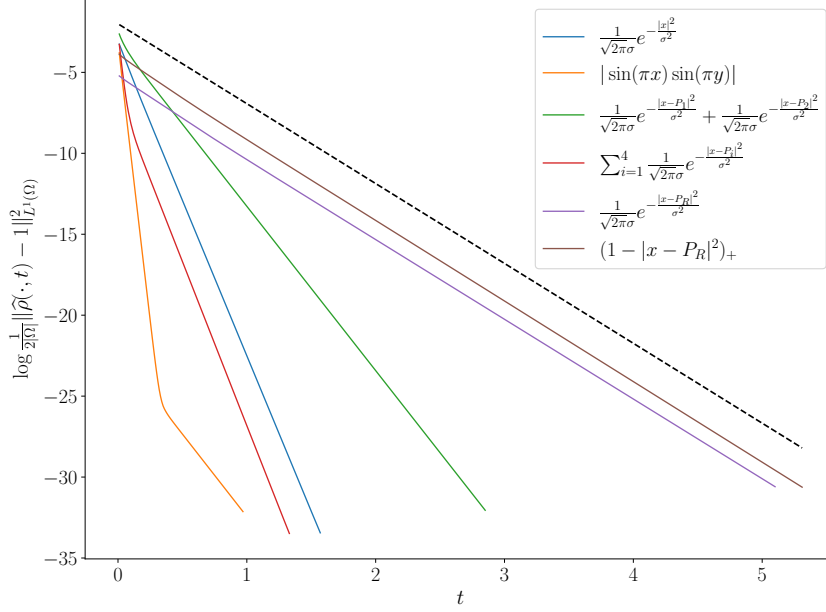
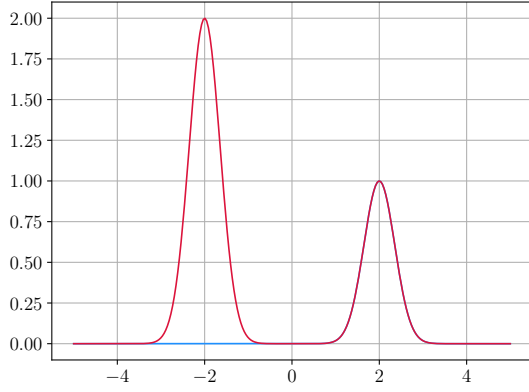


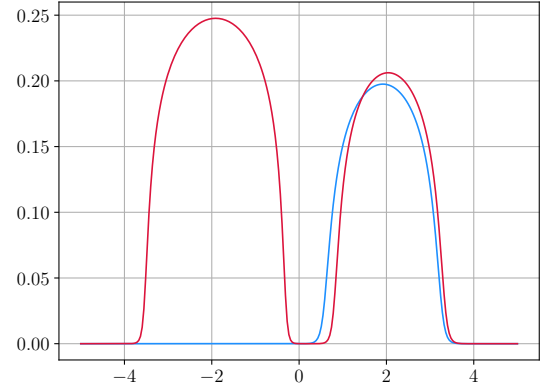
Figure 2.9: The fractional porous medium equation (2.24); exponential decay to the equilibrium solution for different initial data ρ_0 . The computational domain is $\Omega = (-1, 1)^2$, a mesh of $2^7 \times 2^7$ uniformly spaced mesh points was used with the time step taken as $\Delta t = 0.01$, the fractional order is $s = 1/2$, and $x_R = (1, 1)$. The dashed black reference line has slope $-2/C_\Omega$.

with a fractional potential (2.24) with $\mu = 0$; cf. [60, Section 6]. This was demonstrated by numerical simulations in one space dimension in [87]. We show the same phenomenon in a two-dimensional simulation in Figure 2.10 and Figure 2.11. We choose a small constant value of μ and two initial data: $u_1(x) = g(x-2)$ and $u_2(x) = g(x-2) + 2g(x+2)$, where $g(x) \propto e^{-|x|^2/C}$ for a positive constant C . We see in Figure 2.10 and Figure 2.11 that while the chosen initial data are initially ordered, $u_1 \leq u_2$, the order is lost as the solution evolves over time. This fact is due to the non-locality of the fractional Laplacian: when the density u_2 diffuses, one part of it (the one given initially by $g(x-2)$) is dragged towards the other one (given initially by $2g(x+2)$) that has a higher value, and in this way the comparison with u_1 , which is concentrated in part of the domain only, is lost.

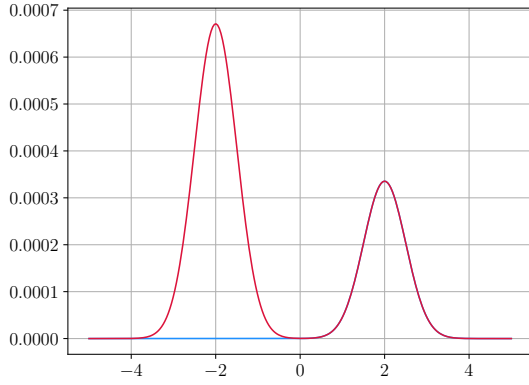
In the end, we highlight some open problems related to the scheme that we developed in Chapter 1. The presence of the upper cut-off parameter L was crucial in the fixed point argument on which the proof, in Lemma 1.11, of the existence of a solution to the fully-discrete scheme was based; and its presence was also essential in the derivation of the uniform bounds with respect to δ and the spatial mesh size stated in Lemma 1.12. While, as was noted in Chapter 1, the precise choice of the upper cut-off parameter L becomes irrelevant in the convergence analysis (provided that L is chosen so that it exceeds the supremum of the initial datum), this independence on L was only shown to hold for the temporally semidiscrete scheme, i.e., after passage to the limit with δ and the spatial discretization parameter has taken place; it is unclear



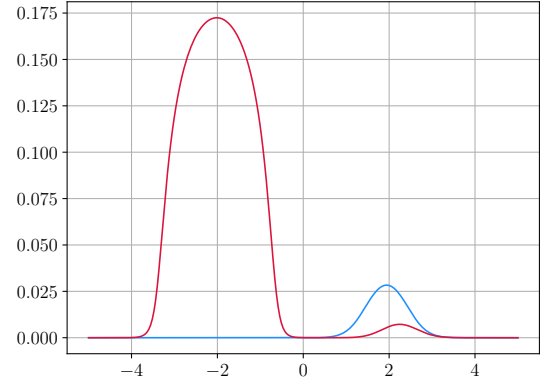
(a) $t = 0$, section $x_1 = x_2$



(b) $t = 4$, section $x_1 = x_2$



(c) $t = 0$, section $x_2 = 0$



(d) $t = 4$, section $x_2 = 0$

Figure 2.10: The fractional porous medium equation (2.24); failure of the comparison principle for fractional order $s = 3/4$. The computational domain is $\Omega = (-R, R)^2$, $R = 5$, $\mu = 10^{-5}$; a uniform mesh of $2^8 \times 2^8$ uniformly spaced mesh points was used with the time step taken as $\Delta t = 0.01$.

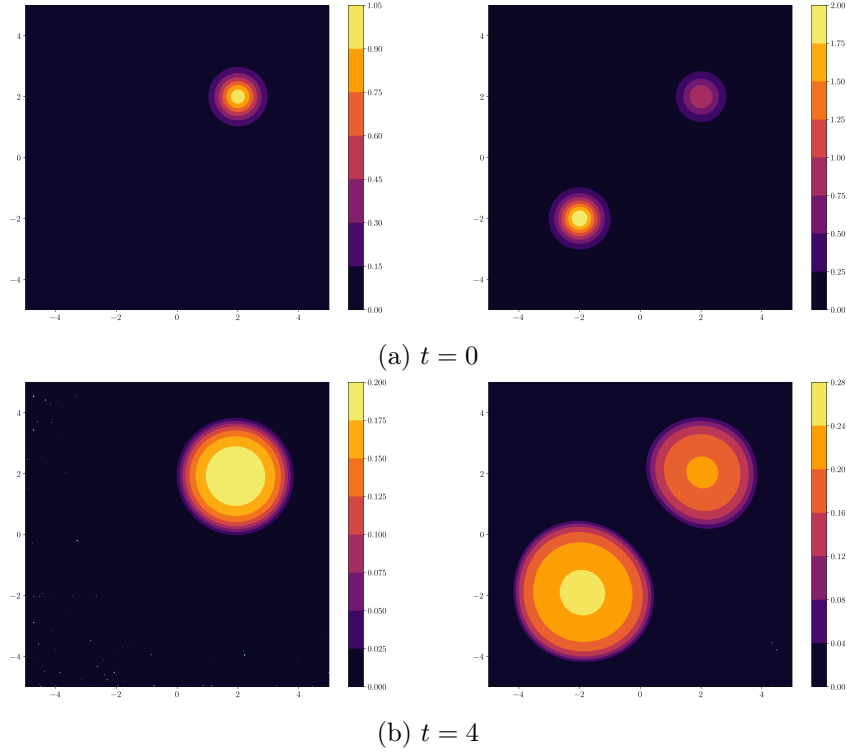


Figure 2.11: The fractional porous medium equation (2.24); failure of the comparison principle for fractional order $s = 3/4$. The computational domain is $\Omega = (-R, R)^2$, $R = 5$, $\mu = 10^{-5}$; a uniform mesh of $2^8 \times 2^8$ uniformly spaced mesh points was used with the time step taken as $\Delta t = 0.01$. On the left the simulation of the equation with initial datum $u_1(x) = g(x - 2)$, $g(x) \propto e^{-|x|^2/C}$ is plotted; on the right the simulation of the equation with initial datum $u_2(x) = g(x - 2) + 2g(x + 2)$ is plotted.

whether a similar independence on L of the solution to the fully discrete scheme holds true. This is however a question that can be explored through numerical simulations. In connection with this an interesting open problem is in fact whether the limits for the spatial discretization parameter $h \rightarrow 0$ and the time step $\Delta t \rightarrow 0$ commute. As was previously noted, from the theoretical point of view the dependence on L in the energy estimate (1.35) in Lemma 1.12 prevents simultaneous passage to the limit in space and time. The proof of independence from L of the semidiscrete-in-time solution, through Lemma 1.16 and Lemma 1.17, is grounded in the properties of the spectral fractional Laplacian $(-\Delta)^s$ and its representation formula. Having said this, we believe that these limits do commute. To support this hypothesis, numerical experiments can be conducted, and our results empirically confirm that the order of taking these limits does not affect the final numerical solution. More precisely, denoting by $\rho_h^{\Delta t}$ the finite element approximation of the solution to problem (1.4) for fixed h and Δt , we computed a series of approximations for $h = 2^{-n}$, $n = 2, \dots, 8$, and $\Delta t = 2^{-k}$, $k = 6, \dots, 12$. We then evaluated the $L^2(\Omega)$ norm of the difference between each approximation $\rho_h^{\Delta t}$ and a reference solution that we denote by $\tilde{\rho}$, defined as the approximation corresponding to the smallest values of the discretization parameters h and Δt , namely $\tilde{\rho} = \rho_{h=2^{-8}}^{\Delta t=2^{-12}}$. By examining the plots in Figures 2.12 and 2.14, we observe that $\|\rho_h^{\Delta t} - \tilde{\rho}\|_{L^2(\Omega)} \rightarrow 0$ as $h \rightarrow 0$ and $\Delta t \rightarrow 0$, regardless of whether the limits are taken simultaneously or sequentially (first in space then time, or vice versa). This supports our intuition that the limits commute in practice, even if the convergence analysis presented above was based on passing to the limit $h \rightarrow 0$, before taking the limit $\Delta t \rightarrow 0$.

An additional interesting question that arises from our analysis, and one that is commonly studied in the context of finite element methods, is the rate of spatial convergence as the spatial discretization parameter h tends to zero. To this end, we tested the method through a series of simulations. Figure 2.13 shows that the observed rate of spatial convergence in $L^2(\Omega)$ norm is quadratic in h , and that the choice of the time step does not influence the spatial speed of convergence.

2.2.2 The fractional Keller–Segel model

In the final part of this chapter, as we indicated earlier, we use our algorithm to computationally explore the fractional Keller–Segel equation. The standard Keller–Segel model is a well-established mathematical model used to describe chemotaxis, that is, the directed movement of cells or organisms in response to chemical gradients. In recent years, there has been significant interest in studying nonlocal generalizations of the model, with the standard Laplacian replaced by the fractional Laplacian; see, for instance, [32, 29, 130] and the references therein. This variant is motivated by the need to model anomalous diffusion, such as Lévy flights or long-range

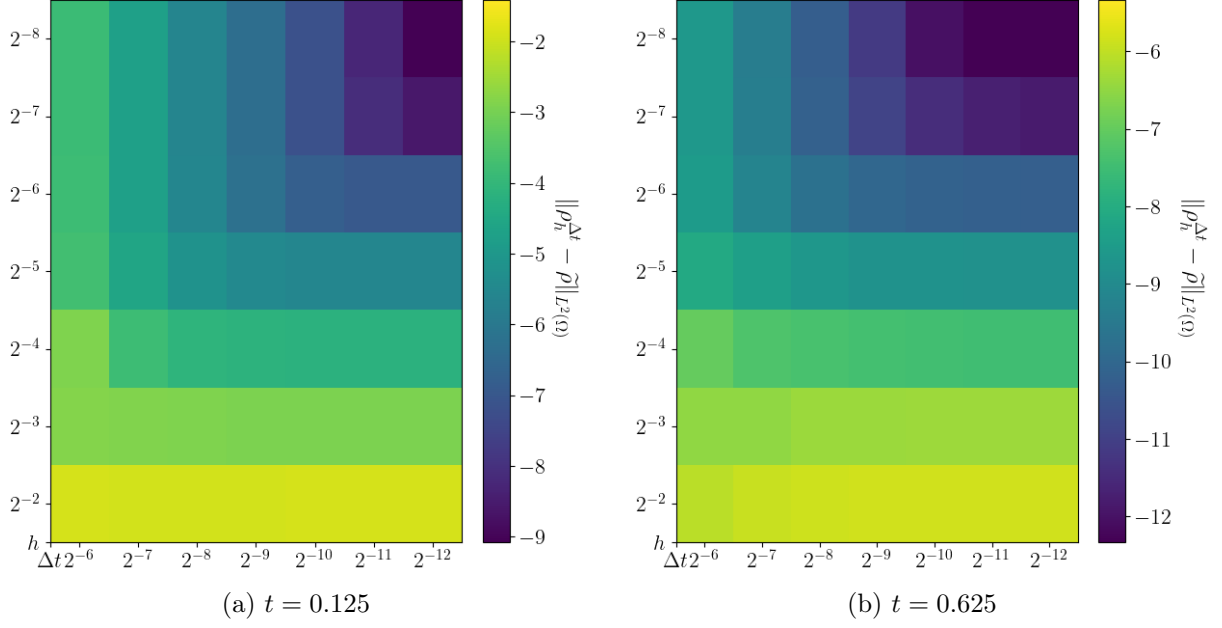


Figure 2.12: Numerical solutions to the fractional porous medium equation (2.24), with passage to the limit for $h \rightarrow 0$ and $\Delta t \rightarrow 0$. The simulations were performed for the fractional order $s = 0.5$ with different values of the spatial discretization parameter $h = 2^{-n}$, $n = 2, \dots, 8$, and different time steps $\Delta t = 2^{-k}$, $k = 6, \dots, 12$. The computational domain is $\Omega = (0, 1)^2$, $\rho_0(x) \propto \exp(-|x|^2/(2\pi\sigma))$, $\sigma = 0.02$. The parabolic regularisation coefficient was $\mu = 0.01$.

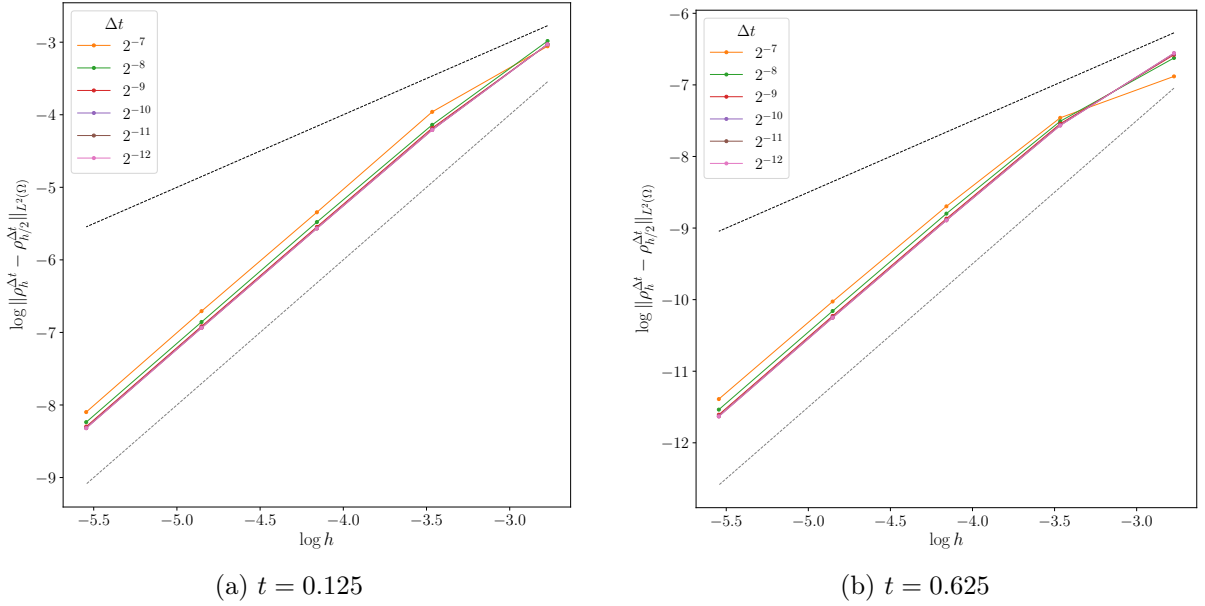
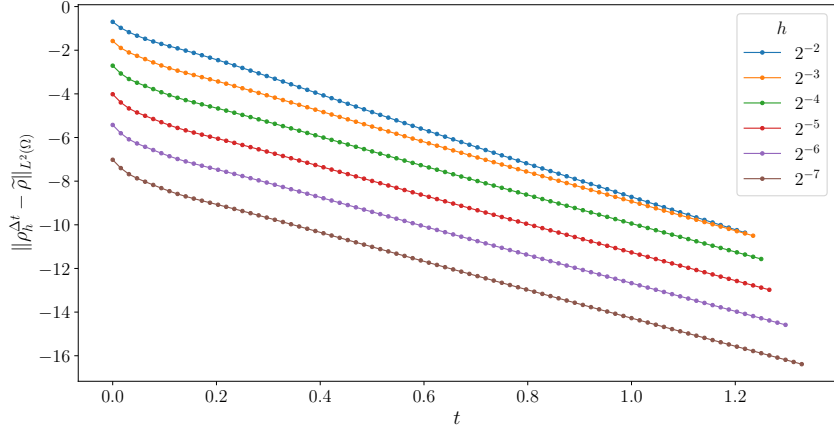
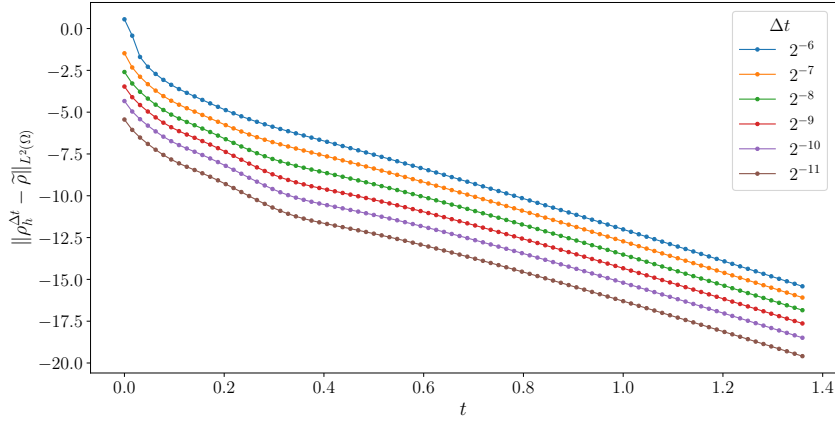


Figure 2.13: Numerical solutions to the fractional porous medium equation (2.24), with convergence in space as $h \rightarrow 0$. The simulations were performed for the fractional order $s = 0.5$, for different values of the spatial discretization parameter $h = 2^{-n}$, $n = 2, \dots, 8$, and different time steps $\Delta t = 2^{-k}$, $k = 6, \dots, 12$. The computational domain is $\Omega = (0, 1)^2$, $\rho_0(x) \propto \exp(-|x|^2/(2\pi\sigma))$, $\sigma = 0.02$. The parabolic regularisation coefficient was $\mu = 0.01$. The black reference line has slope one and the grey reference line has slope two.



(a) $\Delta t = 2^{-12}$



(b) $h = 2^{-8}$

Figure 2.14: Numerical solutions to the fractional porous medium equation (2.24), with passage to the limit for $h \rightarrow 0$ and $\Delta t \rightarrow 0$. The simulations were performed for the fractional order $s = 0.5$ with different values of the spatial discretization parameter $h = 2^{-n}$, $n = 2, \dots, 7$, keeping $\Delta t = 2^{-12}$ fixed, and for different values of time step $\Delta t = 2^{-k}$, $k = 6, \dots, 11$, keeping $h = 2^{-8}$ fixed. The computational domain is $\Omega = (0, 1)^2$, $\rho_0(x) \propto \exp(-|x|^2/(2\pi\sigma))$, $\sigma = 0.02$. The parabolic regularisation parameter was $\mu = 0.01$.

interactions, often observed in biological and ecological systems. The model is given by

$$\frac{\partial \rho}{\partial t} = \Delta \rho - \nabla \cdot (\rho \nabla c), \quad \text{where } (-\Delta)^s c = \rho. \quad (2.31)$$

Blow-up in the context of the Keller–Segel model refers to the unbounded growth of the solution in finite time, signifying the collapse of the population into a singular structure. The conditions under which blow-up occurs are critical for understanding the balance between chemotactic attraction and diffusive dispersion.

For the classical Keller–Segel equation, that is, for $s = 1$, it has been shown that in $\mathbb{R}^d$ blow-up of the solution can occur if the initial mass is larger than a critical value. In the seminal paper [126] blow-up was proved for the classical model in $\mathbb{R}^2$ when the initial mass exceeds a critical threshold, which was later determined in [93], with the result further completed and improved in [35], where it was shown that, given $M := \int_{\Omega} \rho_0 dx$, if $M > 8\pi$ then the density blows up in finite time, while for $M < 8\pi$ blow-up does not take place. Additional information on blow-up profiles was obtained in [123, 173]. In $\mathbb{R}^d$, for $d \geq 3$, the blow-up depends not only on the initial mass of the solution, but also on how the initial mass density is concentrated; we refer to [75] for further details.

For the fractional regime $0 < s < 1$ the study of potential blow-up for ρ is a challenging undertaking. The blow-up conditions for the fractional Keller–Segel model depend, in any number of dimensions $d \geq 1$, not only on the initial mass M , but also on the relative concentration of the initial density. It is in fact known that on $\mathbb{R}^d$, under some initial mass concentration criteria, the solution ceases to exist in finite time; see [32, Proposition 4.2] and [130, Theorem 3.7] for a more general class of models in which non-standard diffusion is also present.

Blow-up results for the fractional Keller–Segel model were previously proved in the literature with the fractional Laplacian defined through its Riesz integral representation on $\mathbb{R}^d$ (4) or with its truncation to a bounded domain in the case of a homogeneous Dirichlet boundary condition. In this case, the novelty of our contribution is in numerically testing the blow-up in the case of a bounded domain with the spectral representation of the fractional Laplacian. In addition, we provide in Proposition 2.6 a proof of existence of solutions to the fractional Keller–Segel model, based on the spectral definition of the fractional Dirichlet Laplacian as presented in (10), that exhibit finite-time blow-up. Let us consider the fractional Keller–Segel model

$$\frac{\partial \rho}{\partial t} = \Delta \rho - \nabla \cdot (\rho \nabla c), \quad \text{where } (-\Delta_D)^s c = \rho, \quad \frac{1}{2} < s < 1, \quad (2.32)$$

together with its weak formulation

$$\begin{aligned} & \text{Find } \rho \in L^2(0, T; V) \text{ with } \frac{\partial \rho}{\partial t} \in L^2(0, T; V') \text{ such that} \\ & \left\langle \frac{\partial \rho}{\partial t}, \phi \right\rangle = - \int_{\Omega} \nabla \rho \cdot \nabla \phi dx + \int_{\Omega} \rho \nabla c \cdot \nabla \phi dx \quad \text{for all } \phi \in V \text{ and a.e. } t \in (0, T], \end{aligned} \quad (2.33)$$

for $V = H^1(\Omega)$, subject to the initial condition $\rho(x, 0) = \rho_0(x)$, where $\rho_0 \in L^\infty(\Omega)$ and $\rho_0(x) \geq 0$ for a.e. $x \in \Omega$ and where

$$(-\Delta_D)^s c = \rho \text{ in } \Omega, \quad \frac{1}{2} < s < 1. \quad (2.34)$$

We note that taking $\phi \equiv 1$ as a test function in (2.33) implies conservation of mass of ρ in time, namely $\frac{d}{dt}M(t) = 0$, with $M(t) = \int_\Omega \rho(x, t) dx$.

Proposition 2.6. *Let Ω be a ball of radius R centred at zero in $\mathbb{R}^d$ with $d = 2, 3$, and let $\frac{1}{2} < s < 1$. Assume that for every nonnegative $\rho_0 \in L^\infty(\Omega)$ problem (2.33) admits a nonnegative weak solution ρ with initial datum ρ_0 . Then, there exists a nonnegative $\rho_0 \in L^\infty(\Omega)$ such that the corresponding solution blows up in finite time.*

Proof. Consider the second moment function $\Phi(t) := \int_\Omega |x|^2 \rho(x, t) dx > 0$. Clearly $0 < \Phi(0) < \infty$. The idea for proving blow-up, that is for example used in [32], is to follow the evolution of the function $\Phi(t)$ and to prove that Φ satisfies a differential inequality of the form

$$\frac{d}{dt}\Phi(t) \leq f(\Phi(t)), \quad (2.35)$$

where f is a continuous nondecreasing function such that $f(0) < 0$. Once we have shown (2.35), we shall define $\Phi^\dagger := \inf\{\Phi > 0 \text{ such that } f(\Phi) = 0\} \in (0, +\infty]$, for any sufficiently smooth solution of (2.32) with initial second moment satisfying $\Phi(0) < \Phi^\dagger$; then, there exists a time $T^\dagger < \infty$ such that $\lim_{t \nearrow T^\dagger} \Phi(t) = 0$. Vanishing of the second moment will then imply blow-up of the solution. Using the weak formulation of our problem (2.33) and integration by parts, we have that

$$\frac{d\Phi}{dt} = 2dM - 2 \int_{\partial\Omega} \rho x \cdot n + 2 \int_\Omega \rho \nabla c \cdot x dx, \quad (2.36)$$

where $M = \int_\Omega \rho(x, t) dx$ and n is the unit outward normal vector to $\partial\Omega$. As the domain Ω is an open ball centred at zero, it follows that $n = x/|x|$ (notice that we could have assumed Ω to be any bounded convex set with the centre of the coordinate system contained in the interior of Ω to ensure that $x \cdot n \geq 0$) and therefore the second term on the right-hand side (2.36) can be discarded.

For the third term on the right-hand side of (2.36) we shall use Lemma A.11, first noticing that

$$\int_\Omega \rho \nabla c \cdot x dx = \int_\Omega (\nabla c \cdot x)(-\Delta_D)^s c dx. \quad (2.37)$$

Using Lemma A.11 on the right-hand side of (2.37), we immediately have

$$\int_\Omega (\nabla c \cdot x)(-\Delta_D)^s c dx \leq -\frac{1}{2}(d-2s) \int_\Omega c(-\Delta_D)^s c dx = -\frac{1}{2}(d-2s) \int_\Omega c \rho dx. \quad (2.38)$$

We now recall the explicit expression for c , which is the solution of (2.34), given by

$$c(x) = \frac{1}{\Gamma(s)} \int_0^\infty \int_\Omega W_t^\Omega(x, y) \frac{1}{t^{1-s}} \rho(y) dy dt, \quad (2.39)$$

where we denote by W_t^Ω the distributional heat kernel for the heat equation on Ω with homogeneous Dirichlet boundary condition (see [57]). We note that the assumption that ρ is nonnegative implies the nonnegativity of c .

We proceed by considering the following auxiliary problem for $\lambda > 1$:

$$(-\Delta_D^{\lambda\Omega})^s \bar{c} = \bar{\rho} \quad \text{in } \lambda\Omega := \{\lambda x, x \in \Omega\},$$

where $\bar{\rho}$ is the natural extension by zero outside Ω , namely $\bar{\rho}(y) = \rho(y)$ if $y \in \Omega$ and $\bar{\rho}(y) = 0$ if $y \notin \Omega$. By Lemma A.13 we have $\bar{c} \rightarrow c$ in $\mathbb{H}^s(\Omega)$ as $\lambda \rightarrow 1$. This implies strong and hence weak convergence in $L^2(\Omega)$. In particular $(\bar{c}, \rho) \rightarrow (c, \rho)$ as $\lambda \rightarrow 1$. Therefore, there exists a $\lambda_1 > 1$ such that $\frac{1}{2}(\bar{c}, \rho) < (c, \rho) < \frac{3}{2}(\bar{c}, \rho)$. Fix a λ such that $1 < \lambda < \lambda_1$; we can then rewrite (2.38) as

$$\begin{aligned} \int_{\Omega} (\nabla c \cdot x) (-\Delta_D)^s c \, dx &\leq -\frac{1}{2}(d-2s) \int_{\Omega} c \rho \, dx = -\frac{1}{2}(d-2s)(c, \rho) \\ &\leq -\frac{1}{4}(d-2s)(\bar{c}, \rho) = -\frac{1}{4}(d-2s) \int_{\Omega} \bar{c} \rho \, dx. \end{aligned}$$

Since $\bar{\rho}$ is equal to zero outside Ω , for $\bar{c}$ we have an expression analogous to (2.39) with $W_t^{\lambda\Omega}$ in place of W_t^Ω . Therefore we have

$$\int_{\Omega} (\nabla c \cdot x) (-\Delta_D)^s c \, dx \leq -\frac{1}{2}(d-2s) \frac{1}{\Gamma(s)} \int_{\Omega} \int_0^\infty \int_{\Omega} \rho(x) \rho(y) W_t^{\lambda\Omega}(x, y) \frac{1}{t^{1-s}} \, dy \, dt \, dx.$$

Now that the distributional Dirichlet heat kernel refers to the domain $\lambda\Omega$, which strictly contains Ω , we can use the exponential bounds that are known to hold for the distributional heat kernel in a domain Ω , which is strictly inside the domain $\lambda\Omega$:

$$c_1 \frac{e^{-|x-y|^2/(c_3 t)}}{t^{d/2}} \leq W_t^{\lambda\Omega}(x, y) \leq c_2 \frac{e^{-|x-y|^2/(c_4 t)}}{t^{d/2}}, \quad x, y \in \Omega \subset \lambda\Omega, \quad t > 0,$$

for positive constants c_1, c_2, c_3 and c_4 (see [57, Theorem 2.4] or [151, Theorem 2.2]). After integration in time,

$$\begin{aligned} \int_0^\infty \frac{1}{t^{1-s}} W_t^{\lambda\Omega}(x, y) \, dt &\simeq \int_0^\infty \frac{1}{t^{\frac{d}{2}+1-s}} e^{-|x-y|^2/t} \, dt \\ &= \frac{1}{|x-y|^{d-2s}} \int_0^\infty e^{-r} r^{-1-s+\frac{d}{2}} \, dr = \Gamma\left(\frac{d}{2} - s\right) \frac{1}{|x-y|^{d-2s}}, \end{aligned}$$

where in the passage from the first line to the second line we used the change of variable $r = |x-y|^2/t$. We then have that

$$\int_{\Omega} (\nabla c \cdot x) (-\Delta)^s c \, dx \leq -C(d-2s) \frac{\Gamma(d/2-s)}{\Gamma(s)} \int_{\Omega} \int_{\Omega} \rho(x) \rho(y) |x-y|^{-(d-2s)} \, dx \, dy,$$

where $C > 0$ is a constant. Therefore, for some positive constant $C_{d,s} > 0$, it follows that

$$\frac{d\Phi}{dt} \leq 2dM + 2 \int_{\Omega} \rho \nabla c \cdot x \, dx \leq 2dM - C_{d,s}(d-2s) \int_{\Omega} \int_{\Omega} \rho(x) \rho(y) |x-y|^{-(d-2s)} \, dx \, dy.$$

Using Hölder's inequality, denoting $\alpha = d - 2s$ and $I_\alpha = \int_\Omega \int_\Omega |x - y|^{-\alpha} \rho(x) \rho(y) \, dx \, dy$, we have

$$\begin{aligned}
M^2 &= \int_\Omega \int_\Omega \rho(x) \rho(y) \, dx \, dy \\
&\leq \left(\int_\Omega \int_\Omega \rho(x) \rho(y) |x - y|^2 \, dx \, dy \right)^{\frac{\alpha}{\alpha+2}} \left(\int_\Omega \int_\Omega \rho(x) \rho(y) |x - y|^{-\alpha} \, dx \, dy \right)^{\frac{2}{\alpha+2}} \\
&= \left(\int_\Omega \int_\Omega \rho(x) \rho(y) (|x|^2 - x \cdot y - y \cdot x + |y|^2) \, dx \, dy \right)^{\alpha/(\alpha+2)} I_\alpha^{\frac{2}{\alpha+2}} \\
&= \left(2M\Phi - 2 \left| \int_\Omega x \rho(x) \, dx \right|^2 \right)^{\alpha/(\alpha+2)} I_\alpha^{\frac{2}{\alpha+2}};
\end{aligned}$$

hence $2^{-\alpha/2} M^{\alpha/2+2} \Phi^{-\alpha/2} \leq I_\alpha$. Therefore, we have in the end

$$\frac{d\Phi}{dt} \leq 2dM - C_{d,s}(d - 2s)M^{\frac{d}{2}-s+2}\Phi^{-\frac{d}{2}+s} \quad (2.40)$$

This means that if at time $t = 0$ we have

$$\Phi(0)^{\frac{d}{2}-s} < \frac{C_{d,s}(d - 2s)M^{\frac{d}{2}-s+2}}{2dM},$$

then the right-hand side of expression (2.40) is strictly negative, and decreases for $t \geq 0$. □

We test in two space dimensions the behaviour of solutions to (2.31) using our numerical approximation of the fractional Laplacian. We explore the blow-up by choosing several initial values ρ_0 , which are all Gaussians $\rho_0(x) \propto \exp(-|x|^2/2\sigma^2)$ with different masses $M = \int_\Omega \rho_0 \, dx$ and variances σ , leading to a range of initial concentrations. Our results are reported in Figure 2.15 and Figure 2.16. For all of our simulations we chose a dynamic time step Δt_n , defined as follows: in a fully discrete approximation (in space and time), if ρ_h^n is the numerical approximation of the solution to (2.31) at time $t_n = \sum_{k=1}^n \Delta t_k$, then the following time step Δt_{n+1} is defined by $\Delta t_{n+1} := 1/\max(\|\rho_h^n\|_{L^\infty(\Omega)}, |\rho_h^n|_{H^1(\Omega)})$. In our simulations numerical blow-up is declared when the adaptive time step Δt becomes smaller than a threshold value $\delta \ll 1$. We observe strong correlation between blow-up and the initial concentration of the density: for two initial data, having the same mass M , blow-up can happen or not depending on the extent to which the density is concentrated at the origin. Secondly, we notice that blow-up is more likely to occur for small values of the fractional order $s \in (1/2, 1)$.

Our numerical findings bolster what is theoretically known for the fractional Keller-Segel model on $\mathbb{R}^d$ and what we proved in Proposition 2.6. However, as we said before, a rigorous proof of a convergence for a numerical scheme is a more delicate issue, which will be further discussed in the Conclusion as a future potential open problem, together with a possible strategy for addressing the challenge.

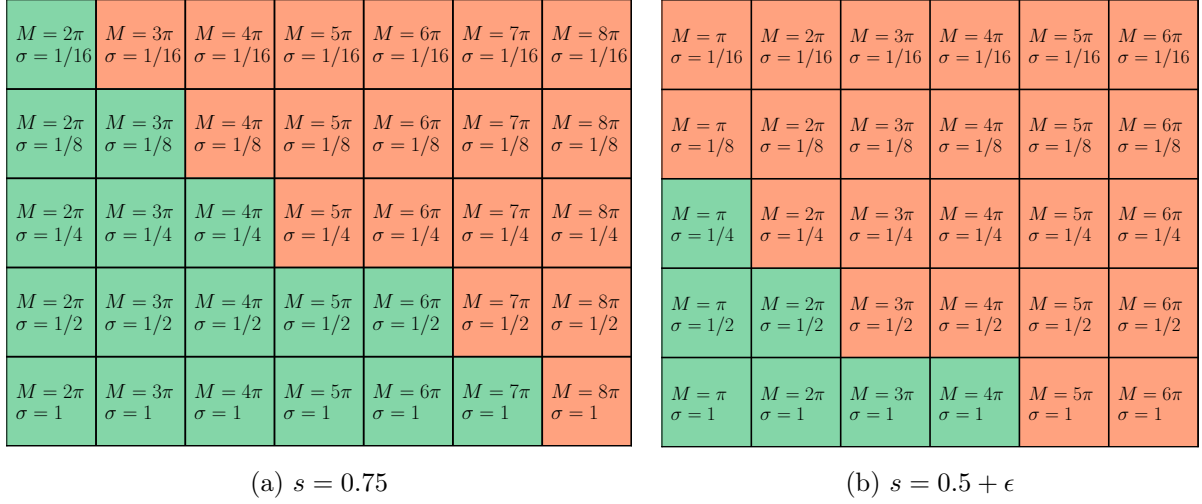


Figure 2.15: The fractional Keller–Segel model (2.31); blow-up, depending on mass and concentration of the initial datum. The numerical tests were performed on the unit disc $\Omega = B_1(0)$; a uniform mesh of 37325 nodes was used for two different fractional orders, $s = 0.75$ in (a) and $s = 0.5 + \epsilon$, $\epsilon = 10^{-12}$ in (b), with different initial data having different masses M and concentrations, given by the parameter σ . Each cell corresponds to a numerical simulation in which either there is no numerical blow-up (green cell) or numerical blow-up occurs (orange cell). The threshold value for numerical blow-up was set to $\delta = 10^{-7}$.

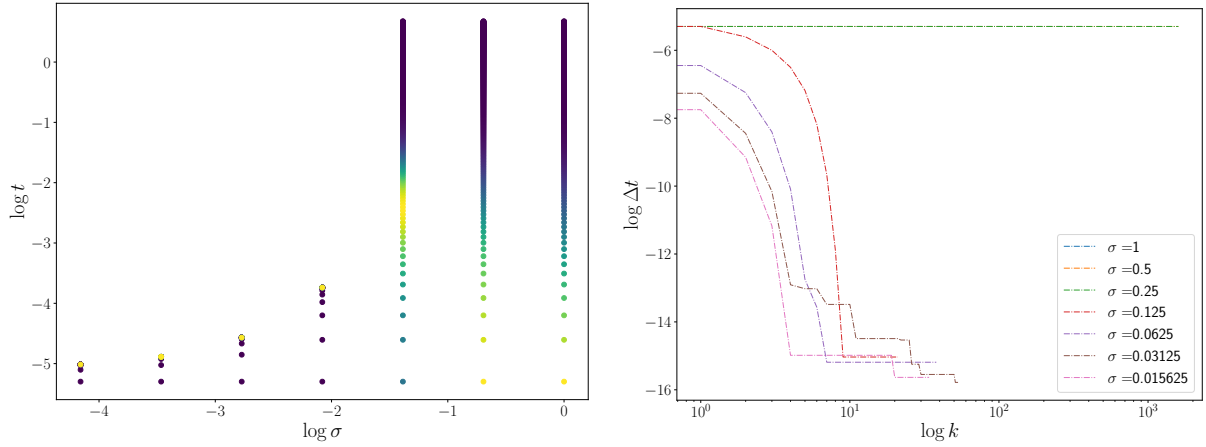


Figure 2.16: The fractional Keller–Segel model (2.31); blow-up depending on the concentration of the initial datum. Numerical tests were performed on the unit disc $\Omega = B_1(0)$; a uniform mesh of 37325 mesh points was used for fractional order $s = 0.75$, with initial data having the same mass $M = 4\pi$ and different concentrations, given by the parameter σ . The threshold value for numerical blow-up was set to $\delta = 10^{-7}$.

I have no idea where this will lead us, but I have a definite feeling it will be a place both wonderful and strange.

David Lynch (1946– 2025), “Twin Peaks”

3

Extended porous medium models with fractional pressure

We now investigate extended models for which a similar scheme to the one that we have presented in Chapter 1 can be proposed. The equations that we will consider are still of porous medium type with a fractional pressure; however, they allow for different fractional operators in place of the fractional Laplacian appearing in equation (1.2). Through these model, we try to understand what would happen if, instead of using the spectral definition of the fractional Laplacian, one adopted a similar definition for another differential operator. These problems constitute a natural extension of the theoretical and computational framework developed previously, and we show that they exhibit interesting features from a modelling perspective.

In the first place, we present a set of assumptions on the class of differential operators for which, with appropriate care and some restrictive hypotheses, the previous scheme can be generalised. Let us consider a linear second-order partial differential operator $\mathcal{L}$, that we assume to be uniformly elliptic, nonnegative, densely defined and self-adjoint in $L^2(\Omega)$. Similarly to what we did for the Laplacian, since we assume to be working on a bounded domain Ω , we pair the operator $\mathcal{L}$ with some boundary conditions on the boundary $\partial\Omega$, meaning that we will consider $\mathcal{L}$ applied to functions under the constraint that a boundary condition holds. Thus, consider $\mathcal{B}(\cdot) = 0$ as a boundary condition and let $\mathcal{L}_{\mathcal{B}}$ denote the differential operator $\mathcal{L}$ paired with a boundary condition $\mathcal{B}$. Let $\{e^{-t\mathcal{L}_{\mathcal{B}}}\}_{t \geq 0}$ be the heat semigroup associated to $\mathcal{L}_{\mathcal{B}}$ and $W_t(x, y)$ the corresponding heat kernel: $e^{-t\mathcal{L}_{\mathcal{B}}}u(x)$ solves the generalised heat equation

$$\begin{cases} \frac{\partial w}{\partial t} = -\mathcal{L}w & \text{in } \Omega \times (0, \infty), \\ w(x, 0) = u(x) & \text{in } \Omega, \\ \mathcal{B}(w) = 0 & \text{on } \partial\Omega \times (0, \infty). \end{cases} \quad (3.1)$$

The main assumption that we require is that the operator $\mathcal{L}_{\mathcal{B}}$ is L^∞ -contractive, meaning that, if $\{e^{-t\mathcal{L}_{\mathcal{B}}}\}_{t \geq 0}$ is the heat semigroup associated to $\mathcal{L}_{\mathcal{B}}$, then

$$\|e^{-t\mathcal{L}_{\mathcal{B}}}f\|_{L^\infty(\Omega)} \leq \|f\|_{L^\infty(\Omega)}, \quad \text{for every } f \in L^\infty(\Omega). \quad (3.2)$$

If the semigroup $\{e^{-t\mathcal{L}_{\mathcal{B}}}\}_{t \geq 0}$ is both positive and L^∞ -contractive, it is called *sub-Markovian*. Roughly speaking, condition (3.2) means that the operator $\mathcal{L}$ is “dissipative”: the solution to (3.1) dissipates in time in terms of the $L^\infty(\Omega)$ norm. L^∞ -contractivity holds very often for general elliptic operators with real coefficients, paired with standard boundary conditions, such as Dirichlet or Neumann (we refer the reader to [147, Chapter 4]).

Notice that L^∞ -contractivity would follow if the heat kernel of $\mathcal{L}_{\mathcal{B}}$ had a Gaussian upper bounded global in time, that is

$$W_t(x, y) \leq c_1 \frac{e^{-|x-y|^2/(c_2 t)}}{t^{\frac{d}{2}}}, \quad x, y \in \Omega, \quad t > 0, \quad (3.3)$$

for some positive constants c_1, c_2 . However, (3.3) does not always hold: for example, for $-\Delta_N$ a Gaussian upper bound on the heat kernel holds only for short times and the heat kernel is then only bounded in x, y and t as $t \rightarrow \infty$. In general, one could have the bound in (3.3) only on a finite time interval $(0, T)$, $T > 0$, with exponential growth of the upper bound on the kernel, i.e.

$$W_t(x, y) \leq c_1 \frac{e^{-|x-y|^2/(c_2 t)}}{t^{\frac{d}{2}}} e^{at}, \quad x, y \in \Omega, \quad t \in (0, \infty),$$

for some $a > 0$ (see [136, Theorem 4 and 7] and for a broader discussion on Gaussian upper bounds we refer to [147, Chapter 6]). At this stage we also notice that

$$\int_{\Omega} W_t(x, y) dy = e^{-t\mathcal{L}_{\mathcal{B}}}1(x),$$

where $1(x)$ stands for the function that is identically equal to 1 for $x \in \Omega$, and hence the heat kernel has in general mass smaller than or equal to 1, i.e.

$$\int_{\Omega} W_t(x, y) dy \leq 1. \quad (3.4)$$

The prototype of such a differential operator for us is

$$\mathcal{L}u = -\operatorname{div}(A(x)\nabla u) + Q(x)u, \quad (3.5)$$

for a nonnegative and bounded $Q : \Omega \rightarrow \mathbb{R}$ and a matrix $A(x) \in \mathbb{R}^{d \times d}$ with coefficients $A_{ij}(x) = A_{ji}(x)$ bounded, measurable and satisfying uniform ellipticity, i.e. $\Lambda_1|v|^2 \leq A(x)v \cdot v \leq \Lambda_2|v|^2$, for all $v \in \mathbb{R}^d$ and almost every $x \in \Omega$, for some constants $0 < \Lambda_1 \leq \Lambda_2$. In fact, for such an operator (3.2) holds, as discussed in [147, Theorem 4.9].

Remark 3.1 (Absence of the lower order term and Neumann boundary conditions). We mention the fact that if the lower order term in (3.5) vanishes, that is $Q \equiv 0$ on Ω , then one has that the heat semigroup satisfies a conservation property, that is

$$e^{-t\mathcal{L}_B}1 = 1, \quad \text{for all } t \geq 0,$$

which implies that the kernel has unit mass,

$$\int_{\Omega} W_t(x, y) dy = 1, \quad \text{for all } x \in \Omega$$

(the proof of this fact is due to [147, Theorem 4.17] and the fact that we have already assumed L^∞ -contractivity). If additionally one pairs the operator $\mathcal{L}u = -\operatorname{div}(A(x)\nabla u)$ with a Neumann boundary condition of the form $\mathcal{B}(u) = A(x)\nabla u \cdot n = 0$, where n is the unit outward normal vector to $\partial\Omega$, the heat kernel has a Gaussian upper bound

$$0 \leq W_t(x, y) \leq c_1 \frac{e^{-|x-y|^2/(c_2 t)}}{t^{\frac{d}{2}} \wedge 1}, \quad x, y \in \Omega, \quad t > 0, \quad (3.6)$$

for positive constants c_1, c_2 (see [57, Section 7] or [78, Theorem 3.2.9]).

In the following we will use fractional powers of the class of differential operators that we have considered. Historically, the way in which $\mathcal{L}_B^s$ is defined is through the Balakrishnan formula, introduced in [16], that is given by

$$\mathcal{L}_B^s = \frac{\sin(s\pi)}{\pi} \int_0^\infty \theta^{s-1} (\theta \mathcal{I} + \mathcal{L}_B)^{-1} \mathcal{L}_B d\theta,$$

where $\mathcal{I}$ is the identity operator. Properties of this representation are discussed in detail in [139, Chapter 5].

The expression can be reformulated in terms of the semigroup $\{e^{-t\mathcal{L}_B}\}_{t \geq 0}$ that is generated by $\mathcal{L}_B$,

$$\mathcal{L}_B^s u(x) = \frac{1}{\Gamma(-s)} \int_0^\infty (e^{-t\mathcal{L}_B} u(x) - u(x)) \frac{1}{t^{1+s}} dt. \quad (3.7)$$

The formula is in fact the analogue of (13) for a general operator $\mathcal{L}_B$.

Formulae of these type exist for a negative fractional power of the operator $\mathcal{L}_B$. More precisely $\mathcal{L}_B^{-s}$ is given by

$$\mathcal{L}_B^{-s} = \frac{\sin(s\pi)}{\pi} \int_0^\infty \theta^{-s} (\theta \mathcal{I} + \mathcal{L}_B)^{-1} d\theta \quad (3.8)$$

and similarly

$$\mathcal{L}_B^{-s} u(x) = \frac{1}{\Gamma(s)} \int_0^\infty e^{-t\mathcal{L}_B} u(x) \frac{1}{t^{1-s}} dt. \quad (3.9)$$

Remark 3.2 (Fractional operators and extension problem). For this type of fractional operators there exists a result about an extension problem, analogous to (15), that was proved in [167, Theorem 1.1] as a generalization of the Caffarelli–Silvestre extension problem [55]. Let $u \in$

$\text{Dom}(\mathcal{L}^s)$, consider the solution $U = U(x, y) : \Omega \times [0, \infty) \rightarrow \mathbb{R}$ to the following extension problem

$$\begin{cases} -\mathcal{L}U + \frac{1-2s}{y}U_y + U_{yy} = 0 & \text{in } \Omega \times (0, \infty), \\ U(x, 0) = u(x) & \text{on } \Omega. \end{cases} \quad (3.10)$$

A solution of (3.10) is given by

$$U(x, y) = \frac{1}{\Gamma(s)} \int_0^\infty e^{-t\mathcal{L}}(\mathcal{L}^s u)(x) e^{-\frac{y^2}{4t}} \frac{1}{t^{1-s}} dt,$$

and

$$\lim_{y \rightarrow 0^+} \frac{U(x, y) - U(x, 0)}{y^{2s}} = \frac{\Gamma(-s)}{4^s \Gamma(s)} \mathcal{L}^s u(x) = \frac{1}{2s} \lim_{y \rightarrow 0^+} y^{1-2s} U_y(x, y).$$

Moreover, the following formula holds

$$U(x, y) = \int_\Omega P_y^s(x, z) u(z) dz, \quad \text{with} \quad P_y^s(x, z) = \frac{y^{2s}}{4^s \Gamma(s)} \int_0^\infty W_t(x, z) e^{-\frac{y^2}{4t}} \frac{1}{t^{1+s}} dt;$$

$P_y^s(x, z)$ is called the Poisson kernel. All the previous identities related to the extension problem (3.10) are understood in $L^2(\Omega)$. Notice that, since $\frac{y^{2s}}{4^s \Gamma(s)} \int_0^\infty e^{-\frac{y^2}{4t}} \frac{1}{t^{1+s}} dt = 1$ and we have (3.4), it follows that

$$\int_\Omega P_y^s(x, z) dz \leq 1.$$

Moreover if $e^{-t\mathcal{L}}$ has the contraction property in $L^p(\Omega)$, that is

$$\|e^{-t\mathcal{L}} f\|_{L^p(\Omega)} \leq \|f\|_{L^p(\Omega)} \quad \text{for every } f \in L^p(\Omega),$$

then this passes to the Poisson kernel, in the sense that

$$\left\| \int_\Omega P_y^s(\cdot, z) f(z) dz \right\|_{L^p(\Omega)} \leq \|f\|_{L^p(\Omega)}, \quad \text{for all } y \geq 0,$$

(cf. [167, Theorem 2.1]).

We mention [19] for a work in which fractional spectral powers of an operator of the form (3.5) were studied from a numerical perspective to model fractional diffusion, using the extension problem approach.

Let us now specialise the problem for our purposes. Let us denote by $N(\cdot) = 0$ a homogeneous Neumann boundary condition and with $\mathcal{L}_N$ the differential operator $\mathcal{L}$ paired with it. With an operator of the form (3.5), a homogeneous Neumann boundary condition is of the form $N(u) = A(x) \nabla u \cdot n = 0$. If we denote

$$a_{\mathcal{L}_N}(w, v) := \int_\Omega A(x) \nabla w \cdot \nabla v dx + \int_\Omega Q(x) w v dx, \quad (3.11)$$

the pair $(\text{Dom}(\mathcal{L}_N^{1/2}), \mathcal{L}_N)$ is defined as follows:

$$\begin{aligned} \text{Dom}(\mathcal{L}_N^{1/2}) &:= \left\{ u \in H^1(\Omega) : H^1(\Omega) \ni v \mapsto a_{\mathcal{L}_N}(u, v) \right. \\ &\quad \left. \text{is a continuous linear functional on } L^2(\Omega) \right\}, \\ \int_\Omega (\mathcal{L}_N u) v dx &:= a_{\mathcal{L}_N}(u, v), \quad u \in \text{Dom}(\mathcal{L}_N), \quad v \in H^1(\Omega). \end{aligned}$$

We notice now that if $\mathcal{L}_N u = 0$, then one has

$$0 = \int_{\Omega} A(x) \nabla u \cdot \nabla u \, dx + \int_{\Omega} Q(x) u^2 \, dx \geq \Lambda_1 \int_{\Omega} |\nabla u|^2 \, dx,$$

which implies that $\nabla u = 0$ a.e. in Ω , meaning that, since Ω is a domain, if $\mathcal{L}_N u = 0$ then u is constant a.e. in Ω . However, clearly if u is constant a.e. in Ω then $\mathcal{L}_N u = 0$ if and only if $\int_{\Omega} Q(x) \, dx = 0$, which means, by nonnegativity of Q , that $Q(x) = 0$ for a.e. $x \in \Omega$. In summary, we have two cases:

(K0) there exists a subset of Ω with positive measure such that $Q \neq 0$ on that subset, and thus $\text{Ker}(\mathcal{L}_N)$ is trivial;

(K1) $Q = 0$ a.e. in Ω , and thus $\text{Ker}(\mathcal{L}_N)$ is the set of constant functions.

Let us denote by $L_{\diamond}^2(\Omega)$ the orthogonal complement of the kernel of the operator $\mathcal{L}_N$ in $L^2(\Omega)$, namely

$$L_{\diamond}^2(\Omega) = (\text{Ker}(\mathcal{L}_N))^{\perp}; \quad (3.12)$$

the space $L_{\diamond}^2(\Omega)$ is nothing but $L_*^2(\Omega)$ in case (K1) and $L^2(\Omega)$ itself in case (K0). For the following we also define the projection $\Pi_{\diamond} : L^2(\Omega) \rightarrow L_{\diamond}^2(\Omega)$ as

$$v^{\diamond} = \Pi_{\diamond} v := \begin{cases} v & \text{if (K0),} \\ v - \frac{1}{|\Omega|} \int_{\Omega} v \, dx & \text{if (K1).} \end{cases} \quad (3.13)$$

Clearly $\|\Pi_{\diamond} v\|_{L^2(\Omega)} \leq \|v\|_{L^2(\Omega)}$. Notice that $\Pi_{\diamond} v = v^*$ in case (K1) (we recall that v^* is defined through (1.6)) and $\Pi_{\diamond} v = v$ in case (K0). Let us also denote by $H_{\diamond}^1(\Omega)$ the set of $H^1(\Omega)$ functions that belong to $L_{\diamond}^2(\Omega)$, i.e. $H_{\diamond}^1 := H^1(\Omega) \cap L_{\diamond}^2(\Omega)$; if $v \in H^1(\Omega)$ then $\Pi_{\diamond} v \in H^1(\Omega) \cap L_{\diamond}^2(\Omega)$ by the definition (3.13).

We remark that, under the assumptions that we imposed on the operator, $\mathcal{L}_N$ is nonnegative and self-adjoint and there exists an orthonormal basis of $L_{\diamond}^2(\Omega)$ consisting of eigenfunctions ψ_k , $k \geq 1$, of $\mathcal{L}_N$, that correspond to eigenvalues $0 < \mu_1 \leq \mu_2 \leq \dots \nearrow \infty$, namely

$$\begin{cases} \mathcal{L}\psi_k = \mu_k \psi_k & \text{in } \Omega, \\ A(x) \nabla \psi_k \cdot n = 0 & \text{on } \partial\Omega. \end{cases}$$

Therefore, the operator can also be described as

$$\mathcal{L}_N^s u = \sum_{k=1}^{\infty} \mu_k^s u_k \psi_k, \quad u_k := \int_{\Omega} u(x) \psi_k(x) \, dx. \quad (3.14)$$

In order to ensure existence and uniqueness of solutions to elliptic problems of the type $\mathcal{L}_N^s u = f$, we define $\mathcal{H}_{\diamond}^s(\Omega) := \text{Dom}(\mathcal{L}_N^{s/2})$ as the Hilbert space of functions, quotiented with the kernel of $\mathcal{L}_N$ such that (3.14) belongs to $L_{\diamond}^2(\Omega)$, namely

$$\mathcal{H}_{\diamond}^s(\Omega) = \left\{ u(\cdot) = \sum_{k=1}^{\infty} u_k \psi_k(\cdot) \in L_{\diamond}^2(\Omega) : \|u\|_{\mathcal{H}_{\diamond}^s(\Omega)}^2 := \sum_{k=1}^{\infty} \mu_k^s u_k^2 < \infty \right\}. \quad (3.15)$$

One has that

$$\|u\|_{\mathcal{H}_\diamond^s(\Omega)} = \|\mathcal{L}_N^{s/2} u\|_{L^2(\Omega)} \quad \forall u \in \mathcal{H}_\diamond^s(\Omega)$$

and we notice that for $s = 1$

$$\|u\|_{\mathcal{H}_\diamond^1(\Omega)}^2 = (\mathcal{L}u, u) = \int_\Omega A(x) \nabla u \cdot \nabla u \, dx + \int_\Omega Q(x) u^2 \, dx.$$

In case $Q = 0$ a.e. in Ω , by uniform ellipticity one has the equivalence between $\|\cdot\|_{\mathcal{H}_\diamond^1(\Omega)}$ and $|\cdot|_{H^1(\Omega)}$ on the space $\mathcal{H}_\diamond^1(\Omega)$ by the Poincaré inequality. We denote by $\mathcal{H}_\diamond^{-s}(\Omega)$ the dual space of $\mathcal{H}_\diamond^s(\Omega)$.

We also observe that we can express the heat semigroup in terms of the eigenfunctions and eigenvalues as

$$e^{-t\mathcal{L}_N} u(x) = \sum_{k=1}^{\infty} e^{-t\mu_k} u_k \psi_k.$$

Remark 3.3. Let $\{\lambda_k\}_{k \geq 1}$ be the eigenvalues of the self-adjoint elliptic operator induced by the bilinear form

$$a(\phi, \psi) = \int_\Omega \nabla \phi \cdot \nabla \psi \, dx, \quad \phi, \psi \in H^1(\Omega).$$

We can compare $\{\lambda_k\}_{k \geq 1}$ with the eigenvalues $\{\mu_k\}_{k \geq 1}$ of the bilinear form $a_{\mathcal{L}_N}(\cdot, \cdot)$, defined in (3.11). For ϕ with $\|\phi\|_{L^2(\Omega)} = 1$ we have

$$\begin{aligned} a_{\mathcal{L}_N}(\phi, \phi) &= \int_\Omega A(x) \nabla \phi \cdot \nabla \phi \, dx + \int_\Omega Q(x) \phi^2 \, dx \geq \Lambda_1 \int_\Omega \nabla \phi \cdot \nabla \phi \, dx + \inf_{x \in \Omega} Q(x) \\ &\geq \Lambda_1 a(\phi, \phi) + \inf_{x \in \Omega} Q(x), \end{aligned}$$

where Λ_1 is the uniform ellipticity constant of the operator (3.5).

Using the version of Courant-Fisher min-max theorem for self-adjoint operators on Hilbert spaces (see [149, Theorem XIII.1 and XIII.2]), having assumed that $\{\lambda_k\}_{k \geq 1}$ and $\{\mu_k\}_{k \geq 1}$ are ordered, we have then that

$$\mu_k \geq \Lambda_1 \lambda_k + \inf_{x \in \Omega} Q(x).$$

In order to proceed further we introduce an assumption on the elliptic regularity of the operator $\mathcal{L}_N$. We shall assume from now on that for the operator $\mathcal{L}_N$ elliptic regularity of order $\alpha \in (0, 1]$ holds. Specifically, if $T_{\mathcal{L}_N} : \mathcal{H}_\diamond^{-1}(\Omega) \rightarrow \mathcal{H}_\diamond^1(\Omega)$ is the operator defined for $F \in \mathcal{H}_\diamond^{-1}(\Omega)$ as the solution to

$$a_{\mathcal{L}_N}(T_{\mathcal{L}_N} F, v) = (F, v), \quad \text{for all } v \in \mathcal{H}_\diamond^1(\Omega),$$

(which exists and it is unique by the Lax-Milgram theorem and the assumptions of uniform ellipticity and boundedness that we have already set for $\mathcal{L}$), we assume that, for $r \in (0, \alpha]$, $T_{\mathcal{L}_N}$ is a bounded map of $\mathcal{H}^{-1+r}(\Omega)$ into $\mathcal{H}^{1+r}(\Omega)$. Elliptic regularity is required to obtain convergence rates for the finite element approximation of fractional powers of the general operator $\mathcal{L}_N$. We remark that, for example, elliptic regularity of order $\alpha = 1$ will hold if $\mathcal{L}_N$ has sufficiently smooth

coefficients and if Ω is convex, or if $\mathcal{L}_N$ has sufficiently smooth coefficients and the boundary of the domain is $C^{1,1}$; however the latter is not the case if we work, as we will, with polygonal and polyhedral domains.

Finally, let us now consider the following more general diffusion problem

$$\begin{cases} \frac{\partial \rho}{\partial t} = \Delta \rho - \nabla \cdot (\rho A(x) \nabla c), \\ -\mathcal{L}_N^s c = \rho^\diamond. \end{cases} \quad (3.16)$$

We restrict the range of s to $(1/2, 1)$; this assumption will be crucial for the convergence of the whole finite element approximation for this extended evolutionary problem.

We need to pair the problem (3.16) with some boundary conditions and an initial condition. The expression is slightly different from the one of (1.4), in particular the boundary conditions have to take into account in this case the general form of the operator $\mathcal{L}$ (3.5). As in Chapter 1, we assume that $\Omega \subset \mathbb{R}^d$ is a bounded open Lipschitz domain and additionally convex, and for ease of triangulating Ω , we shall confine ourselves to the case when Ω is a convex polytopal Lipschitz domain in $\mathbb{R}^d$, $d = 2, 3$. The problem that we consider is the following:

$$\begin{cases} \frac{\partial \rho}{\partial t} = \Delta \rho - \nabla \cdot (\rho A(x) \nabla c) & \text{in } \Omega \times (0, \infty), \\ -\mathcal{L}_N^s c = \rho^\diamond & \text{in } \Omega \times (0, \infty), \\ \partial_n \rho = 0, \partial_{n_A} c = 0 & \text{on } \partial\Omega \times (0, \infty), \\ \rho(x, 0) = \rho_0(x) & \text{for all } x \in \Omega, \end{cases} \quad (3.17)$$

where $\rho_0 \in L^\infty(\Omega)$ is a given nonnegative initial datum, with normalized mass $\frac{1}{|\Omega|} \int_\Omega \rho_0 \, dx = 1$, $\rho^\diamond$ is defined through (3.13), $s \in (1/2, 1)$, n is the unit outward normal vector on $\partial\Omega$ and ∂_{n_A} stands for the normal derivative associated with $\mathcal{L}$,

$$\partial_{n_A} w = A(x) \nabla w \cdot n.$$

We now express the problem (3.17) in its weak formulation. Let $V := H^1(\Omega)$; the weak formulation of the initial-boundary-value problem (3.17) is thus as follows:

$$\begin{aligned} & \text{Find } \rho \in L^2(0, T; V) \text{ with } \frac{\partial \rho}{\partial t} \in L^\infty(0, T; V') \text{ such that} \\ & \left\langle \frac{\partial \rho}{\partial t}, \phi \right\rangle = - \int_\Omega \nabla \rho \cdot \nabla \phi \, dx + \int_\Omega \rho A(x) \nabla c \cdot \nabla \phi \, dx \quad \text{for all } \phi \in V \text{ and a.e. } t \in (0, T], \end{aligned} \quad (3.18a)$$

subject to the initial condition $\rho(x, 0) = \rho_0(x)$, where $\rho_0 \in L^\infty(\Omega)$ and $\rho_0(x) \geq 0$ for a.e. $x \in \Omega$ and where

$$-\mathcal{L}_N^s c = \rho^\diamond \text{ in } \Omega, \quad \partial_{n_A} c = 0 \text{ on } \partial\Omega, \quad s \in (1/2, 1). \quad (3.18b)$$

Notice that c is well defined, as the solution to the fractional equation (3.18b) exists and it is unique by Theorem A.1; we will therefore write $c = -\mathcal{L}_N^{-s} \rho^\diamond$. When we speak of a weak solution to the problem (3.18) we mean a couple ρ and c such that (3.18a) and (3.18b) hold.

We will proceed now with the analysis and discussion of a finite element scheme for the problem (3.18). We will first propose a finite element discretization of the equation similar to the one that we introduced in Chapter 1. We then compute numerical solutions to explore the behaviour of the model and with the results of the simulations we discuss its distinctive features and its analogies with the fractional porous medium equation. Subsequently we address the convergence of the scheme, highlighting the difficulties inherent to this extended setting and identifying a direction for future research.

In the following sections, we will use a consistent part of the notation that has already been introduced in Section 1.2.

3.1 Finite Element Approximation

At first, we need to construct a discrete version of the operator $\mathcal{L}_N^s$ in a similar fashion to (1.20). In order to do this, we simply consider the bilinear form defined in (3.11), which is symmetric, bounded and coercive on $H^1(\Omega) \cap L_\diamond^2(\Omega)$ and we can restrict $a_{\mathcal{L}_N}(\cdot, \cdot)$ to $(V_h \cap L_\diamond^2(\Omega)) \times (V_h \cap L_\diamond^2(\Omega))$. The bilinear form (3.11) gives rise in $V_h \cap L_\diamond^2(\Omega)$ to a discrete orthonormal basis of eigenfunctions that we denote by $\{\psi_k^h\}_{k=1}^{N_h}$ with corresponding positive eigenvalues $0 < \mu_1^h \leq \dots \leq \mu_{N_h}^h$ such that

$$a_{\mathcal{L}_N}(\psi_k^h, v_h) = \mu_k^h(\psi_k^h, v_h) \quad \text{for all } v_h \in V_h \cap L_\diamond^2(\Omega), \quad k = 1, \dots, N_h.$$

We can then define a finite-dimensional counterpart of the fractional power of $\mathcal{L}_N$: for $u_h \in V_h \cap L_\diamond^2(\Omega)$ and $s \in [0, 1]$, we have

$$\mathcal{L}_{N,h}^s u_h := \sum_{k=1}^{N_h} (\mu_k^h)^s \tilde{u}_k^h \psi_k^h \quad \text{with } \tilde{u}_k^h := \int_{\Omega} u_h \psi_k^h \, dx, \quad k = 1, \dots, N_h. \quad (3.19)$$

With ρ_h^0 defined as in Section 1.2, the fully-discrete scheme for the generalised problem (3.18) is the following:

$$\begin{aligned} \text{Let } \rho_{h,\delta,L}^0 &:= \rho_h^0 \in V_h. \text{ For } n = 1, \dots, N, \text{ given } \rho_{h,\delta,L}^{n-1} \in V_h, \text{ find } \rho_{h,\delta,L}^n \in V_h \text{ such that} \\ \int_{\Omega} \pi_h \left(\frac{\rho_{h,\delta,L}^n - \rho_{h,\delta,L}^{n-1}}{\Delta t} \phi_h \right) dx &= - \int_{\Omega} \nabla \rho_{h,\delta,L}^n \cdot \nabla \phi_h \, dx + \int_{\Omega} A(x) \nabla c_{h,\delta,L}^n \cdot \Theta_{\delta}^L(\rho_{h,\delta,L}^n) \nabla \phi_h \, dx \\ &\quad \text{for all } \phi_h \in V_h, \end{aligned} \quad (3.20a)$$

where $c_{h,\delta,L}^n \in V_h \cap L_\diamond^2(\Omega)$ satisfies

$$-(\mathcal{L}_{N,h})^s c_{h,\delta,L}^n = (\beta_0^L(\rho_{h,\delta,L}^n))^{\diamond}, \quad s \in (1/2, 1), \quad (3.20b)$$

where $\beta_0^L(\cdot)$ is the cut-off function defined in (1.12) with $\delta = 0$.

Remark 3.4. The use of the cut-off function $\beta_0^L(\cdot)$ in (3.20b) differs from what has been done in (1.27b). This fact will help us in controlling the $L^2(\Omega)$ norm of $c_{h,\delta,L}^n$ in this more general setting. In fact, notice that (3.20b) implies that

$$\begin{aligned}\|c_{h,\delta,L}^n\|_{L^2(\Omega)}^2 &= \sum_{k=1}^{N_h} (\mu_k^h)^{-2s} ((\beta_0^L(\rho_{h,\delta,L}^n))^{\diamond}, \psi_k^h)^2 \leq (\mu_1^h)^{-2s} \sum_{k=1}^{N_h} ((\beta_0^L(\rho_{h,\delta,L}^n))^{\diamond}, \psi_k^h)^2 \\ &= (\mu_1^h)^{-2s} \|(\beta_0^L(\rho_{h,\delta,L}^n))^{\diamond}\|_{L^2(\Omega)}^2 \leq (\mu_1^h)^{-2s} L^2 |\Omega|.\end{aligned}$$

For $h \rightarrow 0$ we have that $\mu_1^h \rightarrow \mu_1$, therefore for h small enough we can control $c\mu_1 \leq \mu_1^h \leq C\mu_1$ for positive constants c, C (say for example $\frac{1}{2}\mu_1 \leq \mu_1^h \leq \frac{3}{2}\mu_1$). Thus, for h small enough, there exists a constant $C(L, \Omega) > 0$, depending only on L and Ω such that

$$\|c_{h,\delta,L}^n\|_{L^2(\Omega)} \leq C(L, \Omega). \quad (3.21)$$

3.2 Numerical Experiments

From a scientific computing perspective, we first start with some numerical experiments. In our view, the results reported below illustrate the capabilities of this extended class of models. In fact, the most relevant aspect of the family of generalised models (3.16) lies in the features introduced by employing a general elliptic operator of the form $\mathcal{L}u = -\operatorname{div}(A(x)\nabla u) + Q(x)u$. This choice enriches the nonlocal diffusion process that these equations describe. By varying $A(x)$ and $Q(x)$, it is possible to model different spatially heterogeneous configurations, which interact with the nonlocal effects arising from the fractional power of the operator.

From a computational perspective, the algorithm that was described in Chapter 2 can be easily adapted to this case. In fact, the use of rational approximations can still be applied for computing solutions to the problem

$$\mathcal{L}_N^s(u) = f. \quad (3.22)$$

Since the operator $\mathcal{L}_N$ is positive and self-adjoint, a finite element discretization of (3.22) will still have the form

$$XM^s X^{-1}U = F,$$

where the matrix M is diagonal and its diagonal elements are the discrete eigenvalues $\{\mu_k^h\}_{k=1}^{N_h}$ of the finite-dimensional version of $\mathcal{L}_N$, given in (3.19). Once one has an approximation of the endpoints of the interval $[\mu_{min}^h, \mu_{max}^h]$, corresponding to the minimum and maximum eigenvalues of $\mathcal{L}_{N,h}$, a rational approximation of degree n can be easily computed via the minimax algorithm [106]. Then, using a similar expression to (2.13) the finite element approximation of (3.22) can be computed efficiently, with all the computational benefits that were discussed in Chapter 2. Pairing the algorithm with the finite element discretization of the equation leverages its full capabilities.

The advantage of having a fast algorithm in this case allows us to perform simulations with fine meshes, using different choices of $A(x)$ and $Q(x)$.

As we did in Chapter 2, we control the parabolic regularisation term through a parameter $\mu > 0$. Thus, we compute simulations for the equation

$$\frac{\partial \rho}{\partial t} = \mu \Delta \rho - \nabla \cdot (\rho A(x) \nabla c), \quad -\mathcal{L}_N^s c = \rho^\diamond, \quad \frac{1}{2} < s < 1.$$

In Figure 3.1 and Figure 3.2 we report the results of two numerical experiments starting from two different initial data ρ_1, ρ_2 , with the following settings:

- I.a. $\Omega = (-2, 2)^2$, $N_h = 2^8 \times 2^8$, $\Delta t = 0.05$, $s = 0.75$,
- I.b. $A_{11}(x_1, x_2) = 10.0$, $A_{22}(x_1, x_2) = 0.1$, $A_{12}(x_1, x_2) = A_{21}(x_1, x_2) = 0$,
- I.c. $Q(x_1, x_2) = 100|(x_1, x_2)|^2$,
- I.d. $\rho_1 = \exp(-(|x_1 + 1|^2 + x_2^2)/\sigma)$,
 $\rho_2 = \exp(-(|x_1 + 1|^2 + x_2^2)/\sigma) + 3 \exp(-(|x_1 - 1|^2 + x_2^2)/\sigma)$, $\sigma = 0.1$.

We can see that the spatial anisotropy introduced by the matrix $A(x)$ and the confinement introduced by the potential $Q(x)$ couples with the nonlocal interactions, generated by $c = -\mathcal{L}_N^{-s} \rho$. The spreading is stronger along the x direction and slowed down away from the center of the domain. The nonlocality makes the comparison principle fail as we see in Figure 3.1: two initial data, ordered at time $t = 0$ $\rho_1(x_1, 0) \leq \rho_2(x_1, 0)$, are no longer ordered as time advances. If we look at the potential $c_2 = -\mathcal{L}_N^{-s} \rho_2$ in Figure 3.2 we see the effect of using a fractional power of the operator $\mathcal{L}_N$: c is nonvanishing in the region between the two initial concentrations of ρ_2 , and hence the density itself is dragged along the gradient of c_2 , that is nonvanishing in between the concentrations; this explains why the comparison principle fails in this setting.

In Figure 3.3 we report the results of a numerical experiment starting from an initial datum ρ_0 with the following configuration:

- II.a. $\Omega = (-2, 2)^2$, $N_h = 2^8 \times 2^8$, $\Delta t = 0.05$, $s = 0.67$,
- II.b. $A_{11}(x_1, x_2) = 0.1$, $A_{22}(x_1, x_2) = 10.0$, $A_{12}(x_1, x_2) = A_{21}(x_1, x_2) = 0$,
- II.c. $Q(x_1, x_2) = \begin{cases} 100.0 & \text{if } x_2 > 0 \\ 1.0 & \text{if } x_2 < 0 \end{cases}$,
- II.d. $\rho_0 = \exp(-(|x_1 + 1|^2 + x_2^2)/\sigma) + \exp(-(|x_1 - 1|^2 + x_2^2)/\sigma)$
 $+ \exp(-(|x_1 - 1|^2 + |x_2 - 1.95|^2)/(\sigma/2)) + \exp(-(|x_1 + 1|^2 + |x_2 + 1.95|^2)/(\sigma/2))$,
 $\sigma = 0.1$.

The experiment whose results are displayed in Figure 3.3 shows that the choice of $A(x)$ and $Q(x)$ affects the nonlocality introduced by the fractional power of the differential operator $\mathcal{L}_N$. The expression for $Q(x)$ reduces the value of the potential c on the upper part of the domain Ω , where $x_2 > 0$. Therefore, even if equal densities are placed respectively at the positions $x_1 = -1.0, x_2 = -1.95$ and $x_1 = 1.0, x_2 = 1.95$, only the first induces an effect on the part of the density concentrated initially at the point $x_1 = -1.0, x_2 = 0.0$, which becomes higher than the one symmetrically placed in $x_1 = 1.0, x_2 = 0.0$. In fact, we can see that the density at $x_1 = -1.0, x_2 = 0.0$ starts immediately to absorb some of the concentration below it. This effect finds further validation in the fact that, at time $t = 0.1$, the potential c is already present in the bottom left area of the domain, in the region between the two initial concentrations placed along the axis $x_1 = -1.0$. The interactions between the concentrations at $x_1 = 1.0, x_2 = 0.0$ and $x_1 = 1.0, x_2 = 1.95$ are absent up to larger times, when the concentrations have diffused in the upper right region of Ω .

These two experiments illustrate the considerable versatility of the general model for modeling purposes, particularly for those applications that could require spatial dependence of the potential c . The hypotheses on $A(x)$ and $Q(x)$ allow for a variety of configurations, able to take into account many possible spatial effects.

We now investigate the long-time behaviour of the models (3.16). As a matter of fact, we observe that if the function $Q(x)$ is not identically equal to zero, in general the uniform steady state is no longer a (trivial) solution for the model (3.16). We can observe this fact in Figure 3.4: taking $Q(x) = |x|^2$ we see that the numerical solution converges to a non-trivial steady state. Conversely, in Figure 3.5 we observe what happens when $Q = 0$ even in the presence of anisotropy $A(x) \neq I$: we computed simulations for differential initial data, analogously to the ones that we used for the experiments in Figure 2.9: measuring the $L^1(\Omega)$ norm distance between the numerical solution and the uniform distribution, we see that all solutions converge to the constant steady state.

We also observe in Figure 3.5 (the case (K1), $Q(x) = 0$ a.e.) that, for all the initial data that we tested, for large times we see an exponential decay towards the steady state. Moreover, for the two initial data that are the furthest from the equilibrium (the Gaussian and a blob centred at a corner of the square domain Ω) the slope of the decay, quite interestingly, matches what we believe is the sharp estimate of the rate that we proved with (1.74) in Theorem 1.23: $-2/C_\Omega$ for $C_\Omega = 1/\lambda_1$ with λ_1 being the first positive eigenvalue of the Neumann Laplacian. We recall that C_Ω is a lower bound on the logarithmic Sobolev constant, as discussed in Lemma 1.22. Even more interestingly, in the case (K0) (nonvanishing Q) we can make similar observations. The experiments in this case are reported in Figure 3.6 and, since the steady state does not have an explicit formula, we compute the $L^1(\Omega)$ norm of the distance between successive time steps, i.e.

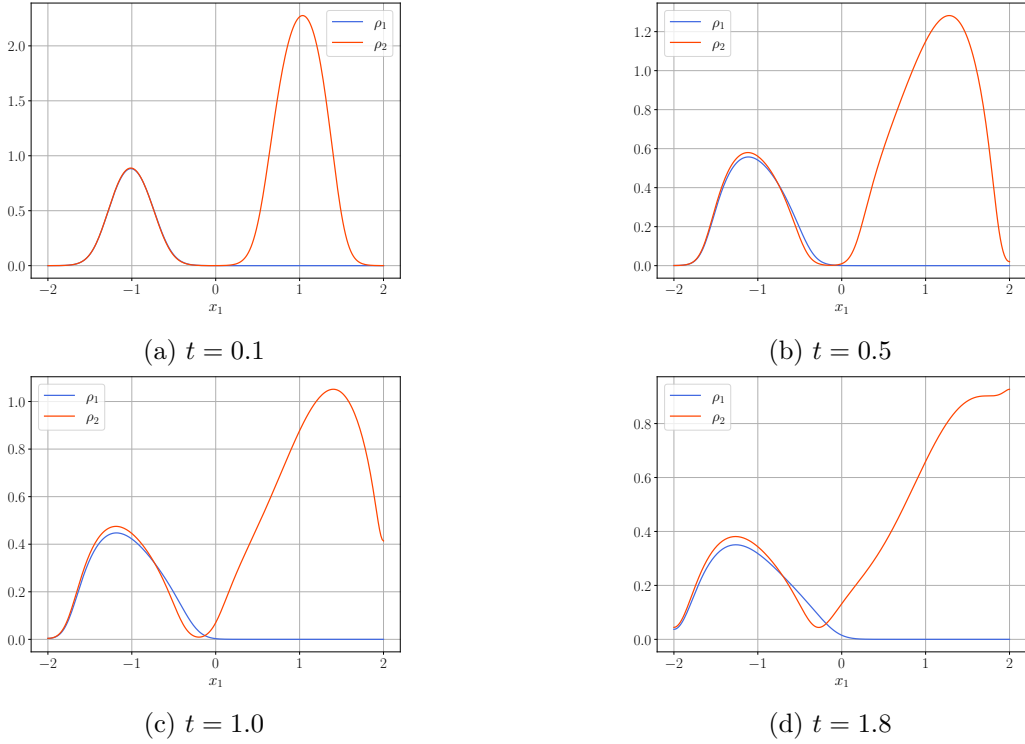


Figure 3.1: Numerical solutions to the generalised porous medium equation with fractional pressure (3.17), cross-section at $x_2 = 0$. The simulations were performed on $\Omega = (-2, 2)^2$ for the fractional order $s = 0.75$ with $h = |\Omega|/(2^8 \cdot 2^8)$, and time step $\Delta t = 0.05$. The matrix $A(x)$ was given by I.b. and the function $Q(x)$ by I.c.. The initial data were I.d.. The parabolic regularisation coefficient was $\mu = 0.01$.

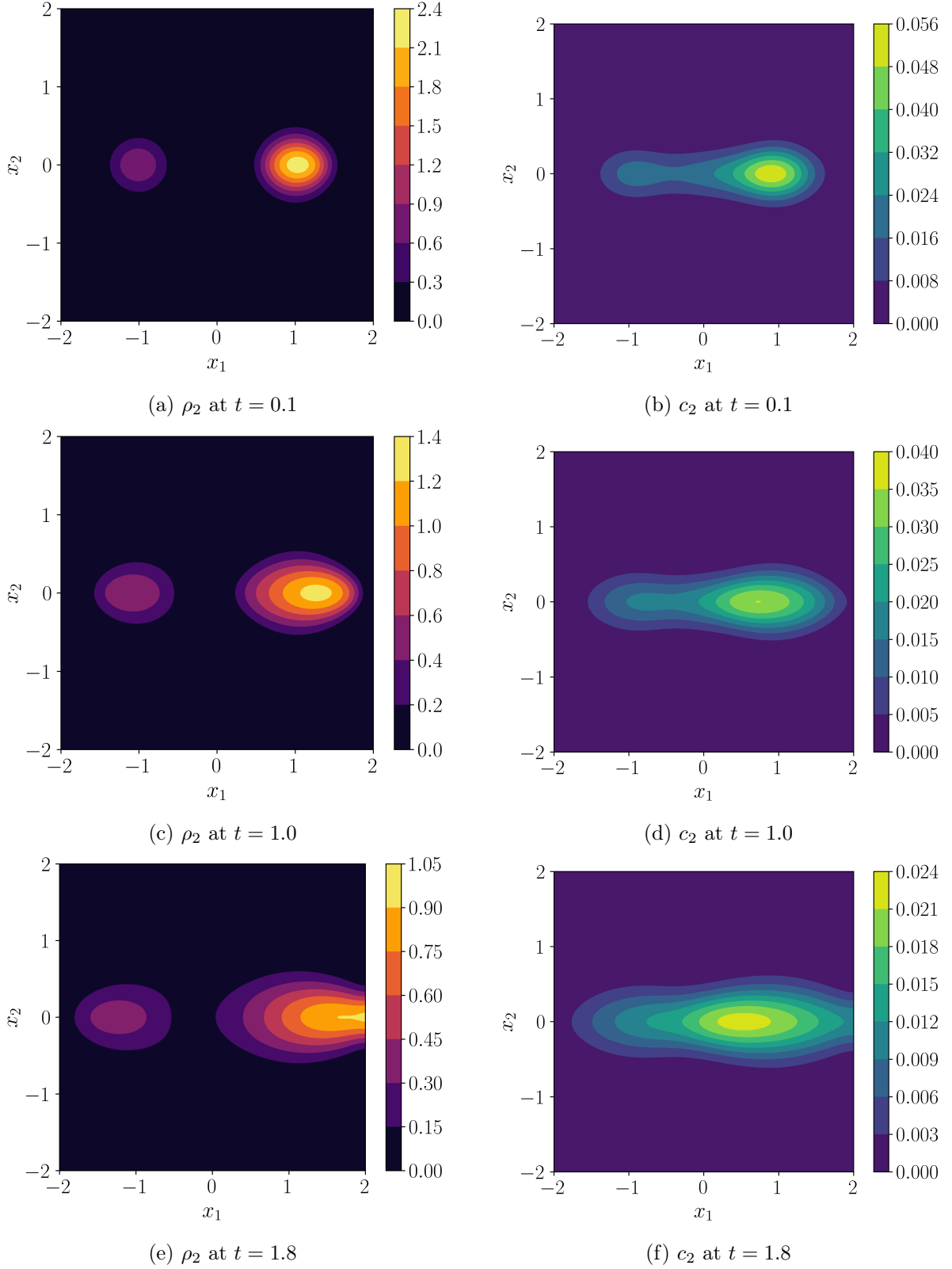


Figure 3.2: Numerical solutions to the generalised porous medium equation with fractional pressure (3.17). The simulations were performed on $\Omega = (-2, 2)^2$ for the fractional order $s = 0.75$ with $h = |\Omega|/(2^8 \cdot 2^8)$, and time step $\Delta t = 0.05$. The matrix $A(x)$ was given by I.b. and the function $Q(x)$ by I.c.. The initial datum was I.d.. The parabolic regularisation coefficient was $\mu = 0.01$.

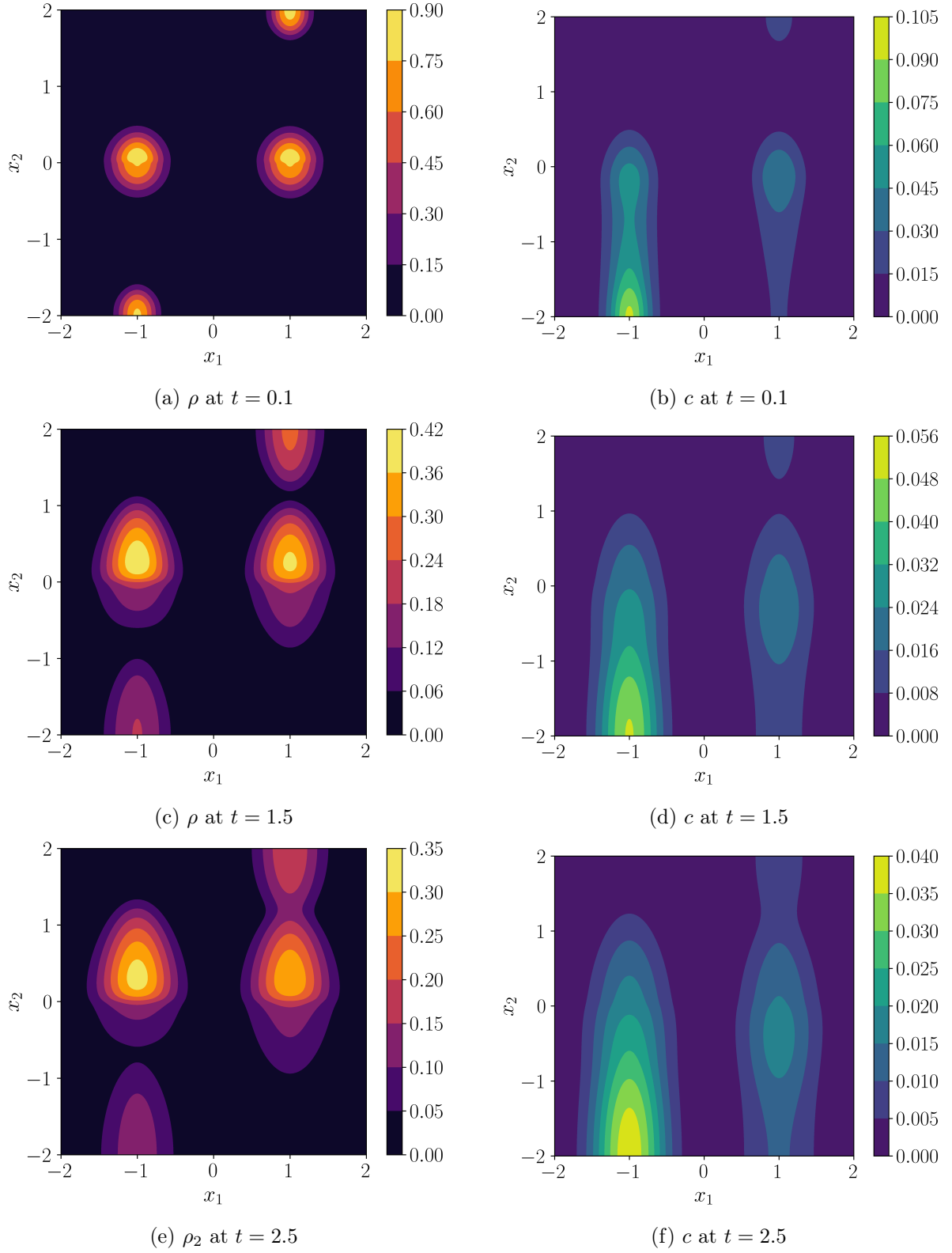


Figure 3.3: Numerical solutions to the generalised porous medium equation with fractional pressure (3.17). The simulations were performed on $\Omega = (-2, 2)^2$ for the fractional order $s = 0.67$ with $h = |\Omega|/(2^8 \cdot 2^8)$, and time step $\Delta t = 0.05$. The matrix $A(x)$ was given by II.b. and the function $Q(x)$ by II.c.. The initial data was II.d.. The parabolic regularisation coefficient was $\mu = 0.01$.

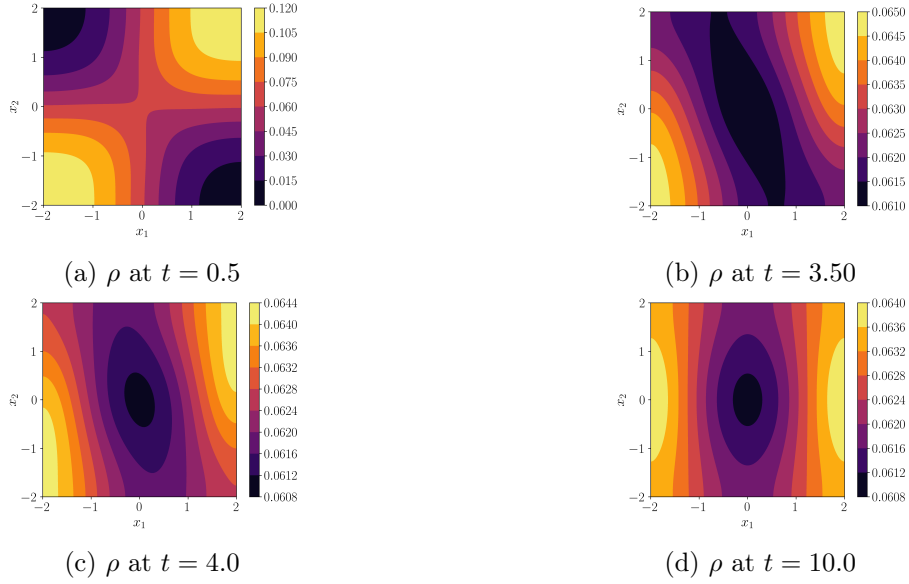


Figure 3.4: Numerical solutions to the generalised porous medium equation with fractional pressure (3.17). The simulations were performed on $\Omega = (-2, 2)^2$ for the fractional order $s = 0.75$ with $h = |\Omega|/(2^7 \cdot 2^7)$, and time step $\Delta t = 0.01$. The matrix $A(x)$ was given by I.b. and the function $Q(x) = |x|^2$. The initial datum was two Gaussians $\rho = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{|x-P_1|^2}{\sigma^2}} + \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{|x-P_2|^2}{\sigma^2}}$, with $P_1 = (1, 1)$ and $P_2 = (-1, -1)$, and $\sigma = 0.4$. The parabolic regularisation coefficient was $\mu = 1$.

$\|\widehat{\rho}(\cdot, t_n) - \widehat{\rho}(\cdot, t_{n-1})\|_{L^1(\Omega)}$. We observe exponential decay and that the presumed sharp rate of $-2/C_\Omega$ is attained for the Gaussian and the blob centred at a corner of the domain.

We shall now proceed with an analysis of convergence of the resulting numerical discretization introduced by (3.20). In analysing the resulting discretization, we will outline the differences and the difficulties with respect to the model treated in Chapter 1 and explain the reasons for the restriction on the fractional order $\frac{1}{2} < s < 1$. Also in this case, we divide the analysis in two stages: firstly taking the limit as $h, \delta \rightarrow 0_+$ and subsequently taking the limit for $\Delta t \rightarrow 0_+$. We show that the first passage to the limit can be carried out in both case (K0) and case (K1), whereas the second, more delicate limit can be handled by a similar argument only in case (K1), that is $Q = 0$ a.e. in Ω . We anticipate that the reason for this restriction lies in the role of an $L^\infty(\Omega)$ bound on the approximated solutions, which constitutes a crucial factor in the argument. Numerical experiments strongly suggest the existence of a uniform control on the L^∞ bound for the solution even in case (K0) (possibly depending on $\|Q\|_{L^\infty(\Omega)}$); such a bound would then immediately allow the same strategy to be applied in case (K0). We leave this limitation as an open problem for future research.

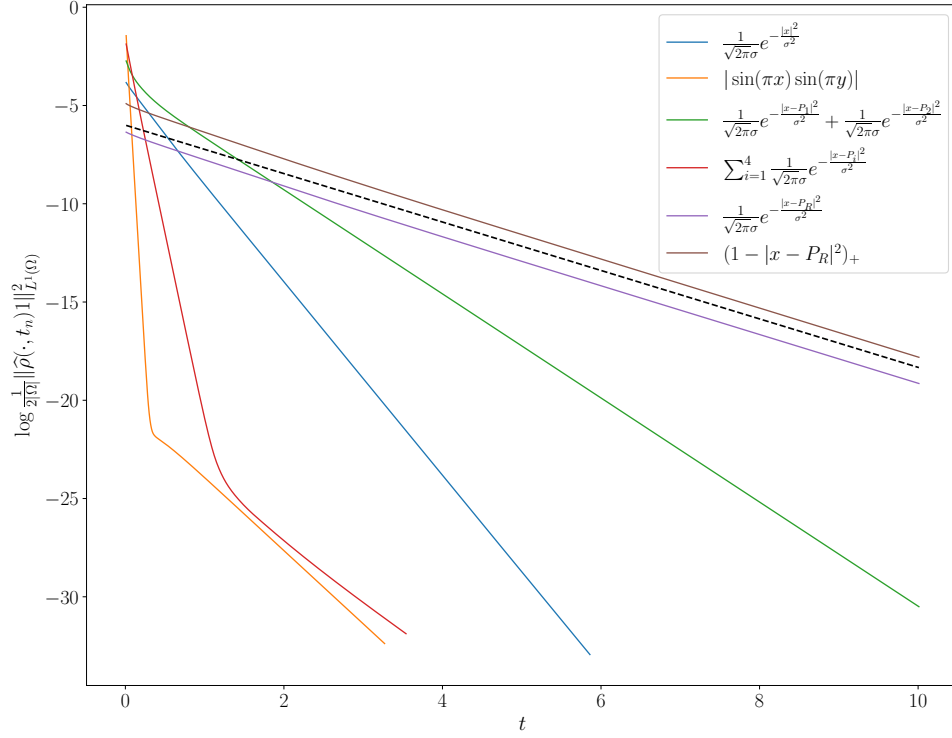


Figure 3.5: Numerical solutions to the generalised porous medium equation with fractional pressure (3.17). The matrix $A(x)$ was given by I.b. and the function $Q(x) = 0$. The simulations were performed on $\Omega = (-2, 2)^2$ for the fractional order $s = 0.75$ with $h = |\Omega|/(2^7 \cdot 2^7)$, and time step $\Delta t = 0.01$. The parabolic regularisation coefficient was $\mu = 1$. Parameters for the initial data were $\sigma = 0.4$, $P_1 = (1, 1)$, $P_2 = (-1, -1)$, $P_3 = (1, -1)$, $P_4 = (-1, 1)$, $P_R = (2, 2)$. The dashed black reference line has slope $-2/C_\Omega$ for $C_\Omega = 1/\lambda_1$, λ_1 the first positive eigenvalue of the Neumann Laplacian.

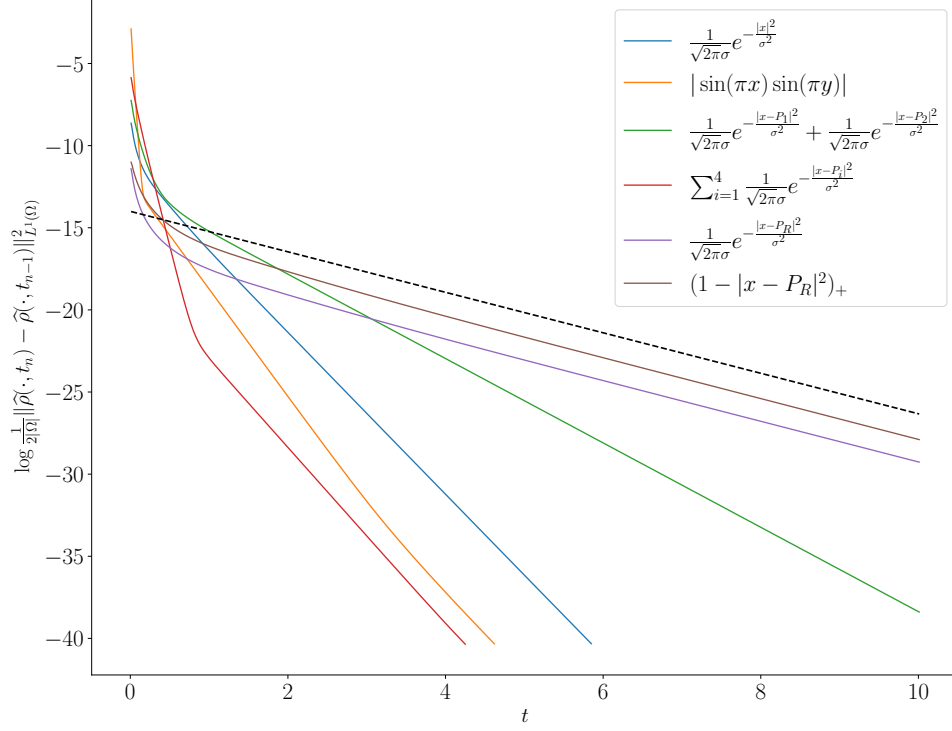


Figure 3.6: Numerical solutions to the generalised porous medium equation with fractional pressure (3.17). The matrix $A(x)$ was given by II.b. and the function $Q(x) = |x|^2$. The simulations were performed on $\Omega = (-2, 2)^2$ for the fractional order $s = 0.75$ with $h = |\Omega|/(2^7 \cdot 2^7)$, and time step $\Delta t = 0.01$. The parabolic regularisation coefficient was $\mu = 1$. Parameters for the initial data were $\sigma = 0.4$, $P_1 = (1, 1)$, $P_2 = (-1, -1)$, $P_3 = (1, -1)$, $P_4 = (-1, 1)$, $P_R = (2, 2)$. The dashed black reference line has slope $-2/C_\Omega$ for $C_\Omega = 1/\lambda_1$, λ_1 the first positive eigenvalue of the Neumann Laplacian.

3.3 Passage to the limit $h, \delta \rightarrow 0_+$

The work in this section consists in showing that, for fixed L and Δt , we can take the limit as $h, \delta \rightarrow 0_+$ in (3.20) and find a family of limit functions ρ_L^n $n = 1, \dots, N$, that satisfies a limit problem. We report below the semidiscrete-in-time problem, that we will reach in the limit $h, \delta \rightarrow 0_+$.

With the definition of $\rho^0 = \rho^0(\Delta t)$ given in Section 1.2 the semidiscrete-in-time approximation of our problem is formulated as follows:

$$\text{Let } \rho_L^0 := \rho^0 = \rho^0(\Delta t). \text{ For } n = 1, \dots, N, \text{ given } \rho_L^{n-1} \in V, \text{ find } \rho_L^n \in V \text{ such that}$$

$$\int_{\Omega} \frac{\rho_L^n - \rho_L^{n-1}}{\Delta t} \phi \, dx = - \int_{\Omega} \nabla \rho_L^n \cdot \nabla \phi \, dx + \int_{\Omega} \beta^L(\rho_L^n) A(x) \nabla c_L^n \cdot \nabla \phi \, dx \quad \text{for all } \phi \in V, \quad (3.23a)$$

subject to the initial condition $\rho_L^0 = \rho^0$, where

$$-\mathcal{L}_N^s c_L^n = (\beta^L(\rho_L^n))^\diamond \quad \text{in } \Omega, \quad s \in (1/2, 1). \quad (3.23b)$$

Lemma 3.5. *For $n = 1, \dots, N$ a solution $\rho_{h,\delta,L}^n \in V_h$ of (3.20a) satisfies the following bound:*

$$\begin{aligned} \int_{\Omega} \pi_h(G_\delta^L(\rho_{h,\delta,L}^n)) \, dx + \Delta t \int_{\Omega} \nabla \rho_{h,\delta,L}^n \cdot \nabla \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) \, dx \\ \leq \int_{\Omega} \pi_h(G_\delta^L(\rho_{h,\delta,L}^{n-1})) + \Delta t \int_{\Omega} A(x) \nabla c_{h,\delta,L}^n \cdot \nabla \rho_{h,\delta,L}^n. \end{aligned} \quad (3.24)$$

Thus, for h small enough, the following bound holds:

$$\max_{n=1,\dots,N} \int_{\Omega} (\rho_{h,\delta,L}^n)^2 \, dx + \frac{1}{\delta} \max_{n=1,\dots,N} \int_{\Omega} \pi_h([\rho_{h,\delta,L}^n]_-^2) \, dx + \Delta t \sum_{n=1}^N \int_{\Omega} |\nabla \rho_{h,\delta,L}^n|^2 \, dx \leq C(L). \quad (3.25)$$

Proof. By taking $\phi_h = \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n))$ as test function in (3.20a), we have that

$$\begin{aligned} \int_{\Omega} \pi_h \left(\frac{\rho_{h,\delta,L}^n - \rho_{h,\delta,L}^{n-1}}{\Delta t} \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) \right) \, dx = - \int_{\Omega} \nabla \rho_{h,\delta,L}^n \cdot \nabla \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) \, dx \\ + \int_{\Omega} A(x) \nabla c_{h,\delta,L}^n \cdot \Theta_\delta^L(\rho_{h,\delta,L}^n) \nabla \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) \, dx. \end{aligned}$$

Hence, by (1.22), it follows that

$$\begin{aligned} \int_{\Omega} \pi_h \left(\frac{\rho_{h,\delta,L}^n - \rho_{h,\delta,L}^{n-1}}{\Delta t} \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) \right) \, dx = - \int_{\Omega} \nabla \rho_{h,\delta,L}^n \cdot \nabla \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) \, dx \\ + \int_{\Omega} A(x) \nabla c_{h,\delta,L}^n \cdot \nabla \rho_{h,\delta,L}^n \, dx. \end{aligned}$$

Next, we bound the left-hand side of this equality from below by using the convexity of G_δ^L , which implies that

$$\begin{aligned} \pi_h \left((\rho_{h,\delta,L}^n - \rho_{h,\delta,L}^{n-1}) \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) \right) &= \pi_h \left((\rho_{h,\delta,L}^n - \rho_{h,\delta,L}^{n-1}) (G_\delta^L)'(\rho_{h,\delta,L}^n) \right) \\ &\geq \pi_h \left(G_\delta^L(\rho_{h,\delta,L}^n) - G_\delta^L(\rho_{h,\delta,L}^{n-1}) \right) \\ &= \pi_h(G_\delta^L(\rho_{h,\delta,L}^n)) - \pi_h(G_\delta^L(\rho_{h,\delta,L}^{n-1})), \end{aligned}$$

and therefore

$$\begin{aligned} \frac{1}{\Delta t} \int_{\Omega} (\pi_h(G_{\delta}^L(\rho_{h,\delta,L})) - \pi_h(G_{\delta}^L(\rho_{h,\delta,L}^{n-1}))) \, dx + \int_{\Omega} \nabla \rho_{h,\delta,L}^n \cdot \nabla \pi_h((G_{\delta}^L)'(\rho_{h,\delta,L}^n)) \, dx \\ \leq \int_{\Omega} A(x) \nabla c_{h,\delta,L}^n \cdot \nabla \rho_{h,\delta,L}^n \, dx. \end{aligned} \quad (3.26)$$

This inequality completes the proof of the first bound (3.24).

In this extended model we have that the right-hand side of inequality (3.26) does not fully contribute ‘constructively’ to the desired bound. In Chapter 1 the advantage of having $\mathcal{L}_N = -\Delta_N$ was making the sign of the right-hand side of (3.26) negative. This fact is not necessarily true for a more general operator $\mathcal{L}_N$, not having the nonnegativity of the finite element approximations; therefore, in this case, another strategy is needed. Using Young’s inequality and the uniform ellipticity assumption of $\mathcal{L}_N$ (recall that $\Lambda_1|v|^2 \leq A(x)v \cdot v \leq \Lambda_2|v|^2$, for all $v \in \mathbb{R}^d$ and almost every $x \in \Omega$, for some constants $0 < \Lambda_1 \leq \Lambda_2$), we have that, for $\varepsilon > 0$,

$$\int_{\Omega} A(x) \nabla c_{h,\delta,L}^n \cdot \nabla \rho_{h,\delta,L}^n \, dx \leq \frac{1}{\varepsilon} C \int_{\Omega} |\nabla c_{h,\delta,L}^n|^2 \, dx + \varepsilon C \int_{\Omega} |\nabla \rho_{h,\delta,L}^n|^2 \, dx, \quad (3.27)$$

where C stands for a real positive constant, independent of h .

We can now use the definition of the bilinear form (3.11), together with the assumption on the positivity and uniform ellipticity of the operator $\mathcal{L}_N$ to have that

$$\begin{aligned} \int_{\Omega} |\nabla c_{h,\delta,L}^n|^2 \, dx &\leq C \int_{\Omega} A(x) \nabla c_{h,\delta,L}^n \cdot \nabla c_{h,\delta,L}^n \, dx \\ &\leq C \left(\int_{\Omega} A(x) \nabla c_{h,\delta,L}^n \cdot \nabla c_{h,\delta,L}^n \, dx + \int_{\Omega} Q(x) (c_{h,\delta,L}^n)^2 \, dx \right) \\ &= C a_{\mathcal{L}_N}(c_{h,\delta,L}^n, c_{h,\delta,L}^n) = C \sum_{k=1}^{N_h} \mu_k^h (\tilde{c}_{h,\delta,L}^n)_k^2, \end{aligned}$$

where $(\tilde{c}_{h,\delta,L}^n)_k = (c_{h,\delta,L}^n, \psi_k^h)$. Therefore

$$\begin{aligned} \int_{\Omega} |\nabla c_{h,\delta,L}^n|^2 \, dx &\leq C(\mathcal{L}_{N,h} c_{h,\delta,L}^n, c_{h,\delta,L}^n) = C(\mathcal{L}_{N,h}^{1-s}(\beta_0^L(\rho_{h,\delta,L}^n))^{\diamond}, \mathcal{L}_{N,h}^{-s}(\beta_0^L(\rho_{h,\delta,L}^n))^{\diamond}) \\ &= C(\mathcal{L}_{N,h}^{1-2s}(\beta_0^L(\rho_{h,\delta,L}^n))^{\diamond}, (\beta_0^L(\rho_{h,\delta,L}^n))^{\diamond}) \\ &= C \sum_{k=1}^{N_h} (\mu_k^h)^{1-2s} (\beta_0^L(\rho_{h,\delta,L}^n))^{\diamond}_k^2 \leq C(\mu_1^h)^{1-2s} \sum_{k=1}^{N_h} (\beta_0^L(\rho_{h,\delta,L}^n))^{\diamond}_k^2 \\ &= C(\mu_1^h)^{1-2s} \|(\beta_0^L(\rho_{h,\delta,L}^n))^{\diamond}\|_{L^2(\Omega)}^2, \end{aligned}$$

with $C > 0$ a real constant, independent of h . By the fact that $s \in (1/2, 1)$, $\mu_1^h \rightarrow \mu_1$ as $h \rightarrow 0$ and by the definition of the cut-off function $\beta_0^L(\cdot)$, one has that, for h small enough there exists a constant, only dependent on L and Ω , that we denote simply by $C(L)$ (absorbing $|\Omega|$ into $C(L)$ and writing $C(L)$ instead of $C(L)|\Omega|$), such that

$$\int_{\Omega} |\nabla c_{h,\delta,L}^n|^2 \, dx \leq C(L). \quad (3.28)$$

Using Corollary 1.9 with $\phi_h = \rho_{h,\delta,L}^n$ and $g = (G_\delta^L)'$, noting that g is strictly monotonically increasing and the inverse g^{-1} is Lipschitz continuous with Lipschitz constant L , we then have that

$$\frac{1}{L} \int_{\Omega} |\nabla \rho_{h,\delta,L}^n|^2 dx \leq \int_{\Omega} \nabla \rho_{h,\delta,L}^n \cdot \nabla \pi_h((G_\delta^L)'(\rho_{h,\delta,L}^n)) dx. \quad (3.29)$$

Therefore, if we pick ε in (3.27) such that $\varepsilon C < L^{-1}$ (say $\varepsilon = (2LC)^{-1}$ for example) and we combine (3.26), (3.27), (3.28), (3.29) we can sum the bounds (3.24) over $n = 1, \dots, m$ to deduce that, for each $m \in \{1, \dots, N\}$,

$$\begin{aligned} \int_{\Omega} \pi_h(G_\delta^L(\rho_{h,\delta,L}^m)) dx + \Delta t \left(\frac{1}{L} - \varepsilon C \right) \sum_{n=1}^m \int_{\Omega} |\nabla \rho_{h,\delta,L}^n|^2 dx &\leq TC(L) + \int_{\Omega} \pi_h(G_\delta^L(\rho_h^0)) dx \\ &= C(L) + \int_{\Omega} \pi_h(G_\delta^L(\rho_h^0)) dx, \end{aligned}$$

where in the last inequality we have simply absorbed T (the final time $T = N\Delta t$) in the constant $C(L)$ as T is a datum of the problem. We can now first bound the first term on the left-hand side of (3.24) using the same consideration as in the proof of Lemma 1.12, showing that

$$\int_{\Omega} \pi_h(G_\delta^L(\rho_{h,\delta,L})) dx \geq \frac{1}{4L} \int_{\Omega} (\rho_{h,\delta,L}^n)^2 dx + \frac{1}{4\delta} \int_{\Omega} \pi_h([\rho_{h,\delta,L}^n]_-^2) dx - C(L)|\Omega|.$$

It follows from (1.26) that $0 \leq G_\delta^L(\rho_{h,\delta,L}^0) \leq C$, where $C = C(L)$ is a positive constant, independent of h and δ , whereby the same is true of $\int_{\Omega} \pi_h(G_\delta^L(\rho_{h,\delta,L}^0)) dx$. From this, the inequality (3.25) directly follows. □

We shall now prove an existence result, similar to Lemma 1.11, using Brouwer's fixed point theorem.

Lemma 3.6. *For any $\Delta t > 0$, for h small enough, given $\rho_{h,\delta,L}^{n-1} \in V_h$, there exists at least one solution $(\rho_{h,\delta,L}^n, c_{h,\delta,L}^n) \in V_h \times (V_h \cap L_\diamond^2(\Omega))$ to (3.20).*

Proof. The proof proceeds in a similar way to the one of Lemma 1.11. We begin by equipping V_h with the inner product $((\cdot, \cdot))$, defined by

$$((\psi_h, \phi_h)) := \int_{\Omega} \pi_h(\psi_h(x)\phi_h(x)) dx, \quad \psi_h, \phi_h \in V_h.$$

Next, we define the function $\mathcal{H} : V_h \rightarrow V_h$ such that, for any $\rho_h \in V_h$,

$$\begin{aligned} ((\mathcal{H}(\rho_h), \phi_h)) &:= \int_{\Omega} \pi_h \left(\frac{\rho_h - \rho_{h,\delta,L}^{n-1}}{\Delta t} \phi_h \right) dx + \int_{\Omega} \nabla \rho_h \cdot \nabla \phi_h dx \\ &\quad - \int_{\Omega} A(x) \nabla c_h \cdot \Theta_\delta^L(\rho_h) \nabla \phi_h dx \quad \text{for all } \phi_h \in V_h, \end{aligned}$$

where $c_h \in V_h \cap L^2_\diamond(\Omega)$ satisfies $-\mathcal{L}_{N,h}^s c_h = (\beta_0^L(\rho_h))^\diamond$. The construction of Θ_δ^L , together with Lemma 1.6, ensures that $\mathcal{H}$ is a continuous mapping. If a solution $\rho_{h,\delta,L}^n$ to (3.20a) exists then it is a zero of $\mathcal{H}$, namely

$$((\mathcal{H}(\rho_{h,\delta,L}^n), \phi_h)) = 0 \quad \text{for all } \phi_h \in V_h.$$

We shall therefore prove that $\mathcal{H}$ has a zero. For contradiction, let us assume that $\mathcal{H}$ has no zero for any $\gamma \in \mathbb{R}_{>0}$ in the ball $B_\gamma = \{\psi_h \in V_h \text{ such that } \|\psi_h\|_{L^2(\Omega)} \leq \gamma\}$. We define the function $\mathcal{E}_\gamma : B_\gamma \rightarrow B_\gamma$ by

$$\mathcal{E}_\gamma(\psi_h) = -\gamma \frac{\mathcal{H}(\psi_h)}{\|\mathcal{H}(\psi_h)\|_{L^2(\Omega)}}.$$

By Brouwer's fixed point theorem $\mathcal{E}_\gamma$ has at least one fixed point ρ_h^γ in B_γ , and this means that $\|\rho_h^\gamma\|_{L^2(\Omega)} = \|\mathcal{E}_\gamma(\rho_h^\gamma)\|_{L^2(\Omega)} = \gamma$. Let c_h^γ be the solution of the equation $-\mathcal{L}_{N,h}^s c_h = (\beta^L(\rho_h^\gamma))^\diamond$ in Ω . Choosing $\phi_h = \pi_h((G_\delta^L)'(\rho_h^\gamma))$ as test function, in a similar fashion as in the proof of Lemma 1.11, by (1.15) and inequality (1.23), together with the trivial equality $\pi_h \rho_h^\gamma = \rho_h^\gamma$, we have that

$$\begin{aligned} ((\mathcal{H}(\rho_h^\gamma), \pi_h((G_\delta^L)'(\rho_h^\gamma)))) &\leq -\frac{\|\mathcal{H}(\rho_h^\gamma)\|_{L^2(\Omega)}}{\gamma} \left(\int_\Omega \left(\frac{(\rho_h^\gamma)^2}{4L} - C(L) \right) dx \right) \\ &= -\frac{\|\mathcal{H}(\rho_h^\gamma)\|_{L^2(\Omega)}}{\gamma} \left(\frac{\gamma^2}{4L} - C(L)|\Omega| \right), \end{aligned}$$

and thus for $\gamma > [4L C(L) |\Omega|]^{1/2}$ we have that

$$((\mathcal{H}(\rho_h^\gamma), \pi_h(G_\delta^L)'(\rho_h^\gamma))) < 0.$$

On the other hand, using the same argument that we applied to obtain (3.24), we deduce that

$$\begin{aligned} ((\mathcal{H}(\rho_h^\gamma), \pi_h(G_\delta^L)'(\rho_h^\gamma))) &\geq \frac{1}{\Delta t} \int_\Omega \pi_h((\rho_h^\gamma - \rho_{h,\delta,L}^{n-1}) \pi_h((G_\delta^L)'(\rho_h^\gamma))) dx + \frac{1}{L} \int_\Omega |\nabla \rho_h^\gamma|^2 dx \\ &\quad - \int_\Omega A(x) \nabla c_h^\gamma \cdot \nabla \rho_h^\gamma dx. \end{aligned} \tag{3.30}$$

For the first term on the right-hand side of (3.30) we can use the convexity of G_δ^L as in Lemma 1.11 to deduce that

$$\frac{1}{\Delta t} \int_\Omega \pi_h((\rho_h^\gamma - \rho_{h,\delta,L}^{n-1}) \pi_h((G_\delta^L)'(\rho_h^\gamma))) dx \geq \frac{1}{\Delta t} \left(\frac{\gamma^2}{4L} - C_1(L)|\Omega| \right) - \frac{1}{\Delta t} \int_\Omega \pi_h(G_\delta^L(\rho_h^{n-1})) dx,$$

for a constant $C_1(L) > 0$, depending on L . For the second and third term on the right-hand side of (3.30) we proceed with a strategy similar to the one applied in the proof of Lemma 3.5.

Using Young's inequality we have

$$\frac{1}{L} \int_\Omega |\nabla \rho_h^\gamma|^2 dx - \int_\Omega A(x) \nabla c_h^\gamma \cdot \nabla \rho_h^\gamma dx \geq \left(\frac{1}{L} - \varepsilon C \right) \int_\Omega |\nabla \rho_h^\gamma|^2 dx - \frac{1}{\varepsilon} C \int_\Omega |\nabla c_h^\gamma|^2,$$

for any $\varepsilon > 0$ and some $C > 0$ and then, choosing $\varepsilon = \frac{1}{2LC}$, by the definition of c_h as a solution of $-\mathcal{L}_{N,h}^s c_h = (\beta^L(\rho_{h,\delta,L}^n))^\diamond$, together with the computations in the proof of Lemma 3.5, that were used to show (3.28), we have

$$\frac{1}{L} \int_{\Omega} |\nabla \rho_h^\gamma|^2 dx - \int_{\Omega} A(x) \nabla c_h^\gamma \cdot \nabla \rho_h^\gamma dx \geq \frac{1}{2L} \int_{\Omega} |\nabla \rho_h^\gamma|^2 dx - C_2(L),$$

for a constant $C_2(L)$, depending on L .

Therefore,

$$((\mathcal{H}(\rho_h^\gamma), \pi_h((G_\delta^L)'(\rho_h^\gamma)))) \geq \frac{1}{\Delta t} \left(\frac{\gamma^2}{4L} - C_1(L)|\Omega| \right) - \frac{1}{\Delta t} \int_{\Omega} \pi_h(G_\delta^L(\rho_h^{n-1})) dx - C_2(L).$$

Thus, for $\gamma > [4L(C_1(L)|\Omega| + \|\pi_h(G_\delta^L(\rho_h^{n-1}))\|_{L^1(\Omega)}) + \Delta t C_2(L)]^{1/2}$ we have

$$((\mathcal{H}(\rho_h^\gamma), \pi_h((G_\delta^L)'(\rho_h^\gamma)))) > 0,$$

and hence we have arrived at a contradiction; therefore the function $\mathcal{H}$ has a zero, which means that at time t_n there exists a solution $\rho_{h,\delta,L}^n \in V_h$ to the fully discrete scheme (3.20a). Having shown the existence of $\rho_{h,\delta,L}^n \in V_h$, the existence of an associated (unique) $c_{h,\delta,L}^n \in V_h \cap L_\diamond^2(\Omega)$ follows from (3.20b). $\square$

As in Chapter 1, we need a result on the convergence in space of the finite element approximation of $\mathcal{L}_N$. Proposition 1.13 has been proved for a general class of elliptic operators $\mathcal{L}$; we refer to [43, Theorem 4.3] and [44, Theorem 6.2] for details. We report here the general statement applicable to our case.

Proposition 3.7 (Convergence of the spatial discretization of the fractional powers of $\mathcal{L}_N$). *Let $\alpha \in (0, 1]$ be the elliptic regularity order of the operator $\mathcal{L}_N$. Suppose that $s \in (1/2, 1)$, $\sigma \in [0, 1]$ and $f \in \mathcal{H}_\diamond^{2\sigma}(\Omega)$. Then, there exists a positive constant C that is independent of h and σ and f such that*

$$\|\mathcal{L}_N^{-s} f - \mathcal{L}_{N,h}^{-s} \Pi_h f\|_{L^2(\Omega)} \leq C\varepsilon(h) \|f\|_{\mathcal{H}_\diamond^{2\sigma}(\Omega)} \quad \text{for all } f \in \mathcal{H}_\diamond^{2\sigma}(\Omega),$$

where

$$\varepsilon(h) = \begin{cases} h^{2\alpha} & \text{if } s + \sigma > \alpha, \\ \log(h^{-1}) h^{2\alpha} & \text{if } s + \sigma = \alpha, \\ \log(h^{-1}) h^{2(s+\sigma)} & \text{if } s + \sigma < \alpha, \end{cases}$$

and Π_h is the $L^2(\Omega)$ projection into the linear space V_h .

Theorem 3.8. *The initial data $\{\rho_h^0\}_{h>0}$ defined in (1.24) are such that, for Δt and L fixed, as $h \rightarrow 0_+$ we have that*

$$\rho_h^0 \rightarrow \rho_L^0 = \rho^0 := \rho^0(\Delta t) \quad \text{strongly in } L^2(\Omega). \quad (3.31)$$

Furthermore, there exists a subsequence of $\{\rho_{h,\delta,L}^n\}_{\delta,h>0}$, a nonnegative function $\rho_L^n \in V = H^1(\Omega)$ and $c_L^n \in H_\diamond^1(\Omega)$ such that the following convergence results hold, for each $n \in \{1, \dots, N\}$, as $\delta, h \rightarrow 0_+$:

$$\nabla \rho_{h,\delta,L} \rightarrow \nabla \rho_L^n \quad \text{weakly in } L^2(\Omega; \mathbb{R}^d), \quad (3.32a)$$

$$\rho_{h,\delta,L}^n \rightarrow \rho_L^n \quad \text{strongly in } L^2(\Omega), \quad (3.32b)$$

$$\Theta_\delta^L(\rho_{h,\delta,L}^n) \rightarrow \beta^L(\rho_L^n)I \quad \text{strongly in } L^2(\Omega; \mathbb{R}^{d \times d}), \quad (3.32c)$$

$$c_{h,\delta,L}^n \rightarrow c_L^n \quad \text{strongly in } L_\diamond^2(\Omega), \quad (3.32d)$$

$$\nabla c_{h,\delta,L}^n \rightarrow \nabla c_L^n \quad \text{weakly in } L_\diamond^2(\Omega; \mathbb{R}^d). \quad (3.32e)$$

Moreover, $\{\rho_L^n\}_{n=1,\dots,N}$ solves the problem (3.23a), $\rho_L^n \geq 0$ a.e. on Ω for all $n = 1, \dots, N$, and, given $\rho_L^0 = \rho^0$ such that $\frac{1}{|\Omega|} \int_\Omega \rho^0 dx = 1$, one has $\frac{1}{|\Omega|} \int_\Omega \rho_L^n dx = 1$ for all $n = 1, \dots, N$.

Proof. The proof of (3.31) proceeds the same way as that of the analogous result (1.36), in the proof of Theorem 1.14, since the initial datum ρ_h^0 for (3.20a) has been chosen as in Section 1.2.

Now, let $n \in \{1, \dots, N\}$. The weak convergence (3.32a) and the strong convergence (3.32b) are implied by the inequality (3.25) and the same considerations as in the proof of Theorem 1.14. The nonnegativity of the limit function ρ_L^n follows from (3.32b) and the second bound in (3.25). Combining the second and third bounds in (3.25) and Lemma 1.7 we have the result (3.32c).

The convergence result (3.32d) can be proved in the following way. We have, by use of the stability inequality (A.3) satisfied by the solution of the fractional Poisson equation, that

$$\begin{aligned} & \|\mathcal{L}_N^{-s}(\beta_0^L(\rho_L^n))^\diamond - \mathcal{L}_{N,h}^{-s}(\beta_0^L(\rho_{h,\delta,L}^n))^\diamond\|_{L^2(\Omega)} \\ & \leq \|\mathcal{L}_N^{-s}((\beta_0^L(\rho_L^n))^\diamond - (\beta_0^L(\rho_{h,\delta,L}^n))^\diamond)\|_{L^2(\Omega)} + \|(\mathcal{L}_N^{-s} - \mathcal{L}_{N,h}^{-s})(\beta_0^L(\rho_{h,\delta,L}^n))^\diamond\|_{L^2(\Omega)} \\ & \leq C\|(\beta_0^L(\rho_L^n))^\diamond - (\beta_0^L(\rho_{h,\delta,L}^n))^\diamond\|_{L^2(\Omega)} + \|(\mathcal{L}_N^{-s} - \mathcal{L}_{N,h}^{-s})(\beta_0^L(\rho_{h,\delta,L}^n))^\diamond\|_{L^2(\Omega)}, \end{aligned}$$

and by (3.32b) and the convergence result stated in Proposition 3.7 we have (3.32d); here C signifies a generic positive constant, independent of δ and h .

To prove (3.32e) we need a uniform bound on the gradient of $c_{h,\delta,L}^n$. This fact, under the assumption of $s \in (1/2, 1)$ and using the equality (3.20b) is a direct consequence, as shown with (3.28) in the proof of Lemma 3.5. Having shown that $\nabla c_{h,\delta,L}^n$ is uniformly bounded in $L^2(\Omega; \mathbb{R}^d)$ as $h, \delta \rightarrow 0_+$, the weak convergence result (3.32e) follows from (3.32d) thanks to the uniqueness of the weak limit.

The arguments for the final passage to the limit as $\delta, h \rightarrow 0_+$ and the conservation of mass ($\frac{1}{|\Omega|} \int_\Omega \rho_L^n(x) dx = \frac{1}{|\Omega|} \int_\Omega \rho^0 dx = 1$ for ρ_L^n , $n = 1, \dots, N$) are the same as in the final part of the proof of Theorem 1.14.

□

3.4 Passage to the limit $\Delta t \rightarrow 0_+$ if $Q = 0$ a.e.

Using the notation, that was introduced in Section 1.3, we can write, (3.23a) summed through $n = 1, \dots, N$ as

$$\begin{aligned} & \text{Find } \rho_L^{\Delta t}(\cdot, t) \in V = H^1(\Omega) \text{ for } t \in (0, T], \text{ such that} \\ & \int_0^T \int_{\Omega} \frac{\partial \rho_L^{\Delta t}}{\partial t} \phi \, dx \, dt = - \int_0^T \int_{\Omega} \nabla \rho_L^{\Delta t, +} \cdot \nabla \phi \, dx \, dt + \int_0^T \int_{\Omega} \beta^L(\rho_L^{\Delta t, +}) A(x) \nabla c_L^{\Delta t, +} \cdot \nabla \phi \, dx \, dt \\ & \text{for all } \phi \in L^1(0, T; V), \end{aligned} \tag{3.33a}$$

subject to the initial condition $\rho_L^{\Delta t}(x, 0) = \rho^0(x)$ for a.e. $x \in \Omega$, where $c_L^{\Delta t, +}(\cdot, t) \in \mathcal{H}_{\diamond}^1(\Omega)$ for all $t \in (0, T]$ and satisfies

$$-\mathcal{L}_N^s c_L^{\Delta t, +}(\cdot, t) = (\beta^L(\rho_L^{\Delta t, +}))^{\diamond}(\cdot, t) \quad \text{in } \Omega, \tag{3.33b}$$

for all $t \in (0, T]$, and $\beta^L(r) := \min\{r, L\}$ for $r \in \mathbb{R}_{\geq 0}$.

We remark that, also in this extended setting, since $(\rho_L^{\Delta t})^{\diamond}$ is equal either to $\rho_L^{\Delta t}$ (in case Q is not a.e. identically zero on Ω) or to $(\rho_L^{\Delta t})^{\diamond} = \rho_L^{\Delta t} - \frac{1}{|\Omega|} \int_{\Omega} \rho_L^{\Delta t} \, dx$ (in case Q is a.e. identically zero on Ω), we have that

$$(\rho_L^{\Delta t})^{\diamond}(\cdot, t) := \rho_L^{\Delta t} - \frac{1}{|\Omega|} \int_{\Omega} \rho_L^{\Delta t} \, dx = \frac{t - t_{n-1}}{\Delta t} (\rho_L^n)^{\diamond}(\cdot) + \frac{t_n - t}{\Delta t} (\rho_L^{n-1})^{\diamond}(\cdot),$$

for $t \in [t_{n-1}, t_n]$ and therefore, as for (1.42), we have

$$\frac{\partial (\rho_L^{\Delta t})^{\diamond}}{\partial t}(\cdot, t) = \frac{(\rho_L^{\Delta t, +})^{\diamond}(\cdot, t) - (\rho_L^{\Delta t, -})^{\diamond}(\cdot, t)}{\Delta t} = \frac{\partial \rho_L^{\Delta t}}{\partial t}(\cdot, t).$$

for $t \in (t_{n-1}, t_n]$

Remark 3.9. We first observe that, in this case, we can still obtain a bound on the $H^1(\Omega)$ seminorm of $c_L^{\Delta t, +}$, dependent on $\rho_L^{\Delta t, +}$. We can do this using the definition of the bilinear form associated to $\mathcal{L}_N$ (3.11), together with the restriction on the fractional order $s \in (1/2, 1)$ and the assumption on the positivity and uniform ellipticity of the operator $\mathcal{L}_N$. In fact, for a constant $C > 0$, we have

$$\begin{aligned} \int_{\Omega} |\nabla c_L^{\Delta t, +}|^2 \, dx & \leq C \int_{\Omega} A(x) \nabla c_L^{\Delta t, +} \cdot \nabla c_L^{\Delta t, +} \\ & \leq C \left(\int_{\Omega} A(x) \nabla c_L^{\Delta t, +} \cdot \nabla c_L^{\Delta t, +} \, dx + \int_{\Omega} Q(x) (c_L^{\Delta t, +})^2 \, dx \right) \\ & = C a_{\mathcal{L}_N}(c_L^{\Delta t, +}, c_L^{\Delta t, +}) = C \sum_{k=1}^{\infty} \mu_k (c_L^{\Delta t, +})_k^2. \end{aligned}$$

Therefore

$$\begin{aligned}
\int_{\Omega} |\nabla c_L^{\Delta t,+}|^2 dx &\leq C(\mathcal{L}_N c_L^{\Delta t,+}, c_L^{\Delta t,+}) = C(\mathcal{L}_N^{1-s}(\beta^L(\rho_L^{\Delta t,+}))^\diamond, \mathcal{L}_N^{-s}(\beta^L(\rho_L^{\Delta t,+}))^\diamond) \\
&= C(\mathcal{L}_N^{1-2s}(\beta^L(\rho_L^{\Delta t,+}))^\diamond, (\beta^L(\rho_L^{\Delta t,+}))^\diamond) \\
&= C \sum_{k=1}^{\infty} \mu_k^{1-2s} (\beta^L(\rho_L^{\Delta t,+}))^\diamond_k^2 \leq C \mu_1^{1-2s} \sum_{k=1}^{\infty} (\beta^L(\rho_L^{\Delta t,+}))^\diamond_k^2 \\
&= C \mu_1^{1-2s} \|(\beta^L(\rho_L^{\Delta t,+}))^\diamond\|_{L^2(\Omega)}^2.
\end{aligned}$$

Therefore, for a positive constant $C > 0$ we have that

$$\int_{\Omega} |\nabla c_L^{\Delta t,+}|^2 dx \leq C \mu_1^{1-2s} L^2 |\Omega|.$$

As we mentioned previously, throughout this section we restrict ourselves to the case (K1), that is $Q = 0$ a.e. in Ω . Indeed, the argument for proving convergence as $\Delta t \rightarrow 0_+$ can only be carried out under a uniform control on the $L^\infty(\Omega)$ norm of the semidiscrete solutions. Thus, we shall now establish a result analogous to Lemma 1.16, namely a bound in time on the $L^\infty(\Omega)$ norm of the solution $\rho_L^{\Delta t}$ in the case $Q = 0$ a.e. in Ω . This fact is an essential property that is crucial in the rest of the analysis, since it allows us to eliminate the dependence on the parameter L and obtain the uniform bounds that are needed for the application of Dubinskii's theorem and its compactness argument. The result is a consequence of the hypotheses that we have made for the operator $\mathcal{L}$, in particular the fact that the operator has been assumed to be sub-Markovian and hence L^∞ -contractive.

Lemma 3.10. *Let $\rho_L^{\Delta t,(\pm)}$ be defined as in (1.40) and assume that $Q = 0$ a.e. in Ω . Then, the following bound holds:*

$$\sup_{t \in (0,T)} \|\rho_L^{\Delta t,(\pm)}(t)\|_{L^\infty(\Omega)} \leq \|\rho_0\|_{L^\infty(\Omega)}. \quad (3.34)$$

Proof. The strategy of the proof starts with a reminiscence of the idea in [56, Section 4.2], which goes back to De Giorgi's approach [58]. However, the procedure here is adapted to the discrete setting to which we are confined. We start by taking a smooth regularisation of the function $\zeta_M : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}$,

$$\zeta_M(z) = \max(z - M, 0),$$

defined as $\zeta_M^\epsilon = \zeta_M * \theta_\epsilon$, where θ_ϵ is a mollifier. By [50, Theorem 4.22] we have that $\zeta_M^\epsilon \rightarrow \zeta_M$ in $L^p([0, K])$, for any $K > 0$, $p \geq 1$ as $\epsilon \rightarrow 0$.

We use $\chi_{[0,t_n]} \zeta_M^\epsilon(\rho_L^{\Delta t,+})$, with $n = 1, \dots, N$, as a test function in (3.33a). We then have

$$\begin{aligned}
\int_0^{t_n} \int_{\Omega} \frac{\partial \rho_L^{\Delta t}}{\partial t} \zeta_M^\epsilon(\rho_L^{\Delta t,+}) dx dt &= - \int_0^{t_n} \int_{\Omega} \nabla \rho_L^{\Delta t,+} \cdot \nabla \zeta_M^\epsilon(\rho_L^{\Delta t,+}) dx dt \\
&\quad + \int_0^{t_n} \int_{\Omega} \beta^L(\rho_L^{\Delta t,+}) A(x) \nabla c_L^{\Delta t,+} \cdot \nabla \zeta_M^\epsilon(\rho_L^{\Delta t,+}) dx dt. \quad (3.35)
\end{aligned}$$

By [50, Lemma 9.1], we have $(\zeta_M^\epsilon)'(z) = (\zeta_M' * \theta_\epsilon)(z)$ in the sense of weak derivatives and therefore, since $\zeta_M'(z) = \chi_{(M, \infty)}(z)$, we have that $(\zeta_M^\epsilon)'(z) \geq 0$. Thus the first term on the right-hand side of (3.35) is

$$-\int_0^{t_n} \int_\Omega \nabla \rho_L^{\Delta t, +} \cdot \nabla \zeta_M^\epsilon(\rho_L^{\Delta t, +}) \, dx \, dt = -\int_0^{t_n} \int_\Omega (\zeta_M^\epsilon)'(\rho_L^{\Delta t, +}) |\nabla \rho_L^{\Delta t, +}|^2 \, dx \, dt \leq 0.$$

For the second term on the right-hand side of (3.35) we have

$$\int_0^{t_n} \int_\Omega \beta^L(\rho_L^{\Delta t, +}) A(x) \nabla c_L^{\Delta t, +} \cdot \nabla \zeta_M^\epsilon(\rho_L^{\Delta t, +}) \, dx \, dt = \int_0^{t_n} \int_\Omega A(x) \nabla c_L^{\Delta t, +} \cdot \nabla H_M(\rho_L^{\Delta t, +}) \, dx \, dt,$$

where $H_M(z) = \int_0^z \beta^L(\omega) (\zeta_M^\epsilon)'(\omega) \, d\omega$. Notice that, because $\rho_L^{\Delta t, +}$ is nonnegative and $(\zeta_M^\epsilon)'(z) \geq 0$, $H_M(\cdot)$ is nonnegative and monotonically increasing.

Notice now that, if $Q = 0$ a.e. in Ω ,

$$\int_\Omega A(x) \nabla c_L^{\Delta t, +} \cdot \nabla H_M(\rho_L^{\Delta t, +}) \, dx = a_{\mathcal{L}_N}(c_L^{\Delta t, +}, H_M(\rho_L^{\Delta t, +})).$$

We highlight that it is precisely in this passage that having $Q = 0$ a.e. in Ω plays a fundamental role: if Q was not identically zero, an additional positive term would appear, preventing the argument from succeeding.

We have that

$$\begin{aligned} \int_\Omega A(x) \nabla c_L^{\Delta t, +} \cdot \nabla H_M(\rho_L^{\Delta t, +}) \, dx &= a_{\mathcal{L}_N}(c_L^{\Delta t, +}, H_M(\rho_L^{\Delta t, +})) \\ &= -(\mathcal{L}_N^{1-s}(\beta^L(\rho_L^{\Delta t, +}))^\diamond, H_M(\rho_L^{\Delta t, +})). \end{aligned} \quad (3.36)$$

We recall that $\{e^{-\tau \mathcal{L}_N}\}_{\tau \geq 0}$ is the heat semigroup associated to the operator $\mathcal{L}_N$. Using that

$$(\beta^L(\rho_L^{\Delta t, +}))^\diamond = (\beta^L(\rho_L^{\Delta t, +}))^* = \beta^L(\rho_L^{\Delta t, +}) - \frac{1}{|\Omega|} \int_\Omega \beta^L(\rho_L^{\Delta t, +}) \, dx$$

and the definition of the heat semigroup (3.1), we then have that

$$e^{-\tau \mathcal{L}_N}(\beta^L(\rho_L^{\Delta t, +}))^\diamond = e^{-\tau \mathcal{L}_N} \beta^L(\rho_L^{\Delta t, +}) - \frac{1}{|\Omega|} \int_\Omega \beta^L(\rho_L^{\Delta t, +}) \, dx.$$

Thus, denoting $\alpha = 2(1 - s)$, using the formula (3.7), we can write

$$\begin{aligned} (\mathcal{L}_N^{\alpha/2}(\beta^L(\rho_L^{\Delta t, +}))^\diamond, H_M(\rho_L^{\Delta t, +})) &= \int_\Omega H_M(\rho_L^{\Delta t, +}(x)) \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty (e^{-\tau \mathcal{L}_N}(\beta^L(\rho_L^{\Delta t, +}))^\diamond(x) \\ &\quad - (\beta^L(\rho_L^{\Delta t, +}))^\diamond(x)) \frac{1}{\tau^{1+\frac{\alpha}{2}}} \, d\tau \, dx \\ &= \int_\Omega H_M(\rho_L^{\Delta t, +}(x)) \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty (e^{-\tau \mathcal{L}_N} \beta^L(\rho_L^{\Delta t, +})(x) - \beta^L(\rho_L^{\Delta t, +})(x)) \frac{1}{\tau^{1+\frac{\alpha}{2}}} \, d\tau \, dx \\ &= \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty \left(\int_\Omega H_M(\rho_L^{\Delta t, +}(x)) e^{-\tau \mathcal{L}_N} \beta^L(\rho_L^{\Delta t, +})(x) \, dx \right. \\ &\quad \left. - \int_\Omega H_M(\rho_L^{\Delta t, +}(x)) \beta^L(\rho_L^{\Delta t, +})(x) \, dx \right) \frac{1}{\tau^{1+\frac{\alpha}{2}}} \, d\tau \\ &= \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty ((e^{-\tau \mathcal{L}_N} \beta^L(\rho_L^{\Delta t, +}), H_M(\rho_L^{\Delta t, +})) - (\beta^L(\rho_L^{\Delta t, +}), H_M(\rho_L^{\Delta t, +}))) \frac{1}{\tau^{1+\frac{\alpha}{2}}} \, d\tau. \end{aligned}$$

Therefore, by plugging the heat kernel in the expression above, we deduce that

$$\begin{aligned}
(\mathcal{L}_N^{\alpha/2}(\beta^L(\rho_L^{\Delta t,+}))^\diamond, H_M(\rho_L^{\Delta t,+})) &= \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty \int_\Omega \left(\int_\Omega W_\tau(x, y) \beta^L(\rho^{\Delta t,+})(x) H_M(\rho^{\Delta t,+})(y) dx \right. \\
&\quad \left. - \beta^L(\rho^{\Delta t,+})(y) H_M(\rho^{\Delta t,+})(y) \right) dy \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau \\
&= \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty \int_\Omega \left(\int_\Omega W_\tau(x, y) (\beta^L(\rho^{\Delta t,+})(x) - \beta^L(\rho^{\Delta t,+})(y)) H_M(\rho^{\Delta t,+})(y) dx \right. \\
&\quad \left. + \beta^L(\rho^{\Delta t,+})(y) H_M(\rho^{\Delta t,+})(y) \left(\int_\Omega W_\tau(x, y) dx - 1 \right) \right) dy \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau \\
&= \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty \int_\Omega \int_\Omega W_\tau(x, y) (\beta^L(\rho^{\Delta t,+})(x) - \beta^L(\rho^{\Delta t,+})(y)) H_M(\rho^{\Delta t,+})(y) dy dx \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau \\
&\quad + \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty \int_\Omega \beta^L(\rho^{\Delta t,+})(y) H_M(\rho^{\Delta t,+})(y) (e^{-\tau \mathcal{L}_N} 1(y) - 1) dy \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau,
\end{aligned}$$

where in the passage from the second to the third line we have added and subtracted the term $\frac{1}{\Gamma(-\alpha/2)} \int_0^\infty \int_\Omega \int_\Omega \beta^L(\rho_L^{\Delta t,+})(y) H_M(\rho^{\Delta t,+})(y) W_t(x, y) dx dy \tau^{-(1+\alpha/2)} d\tau$. By exchanging x and y and using the symmetry of the heat kernel we have also

$$\begin{aligned}
(\mathcal{L}_N^{\alpha/2}(\beta^L(\rho_L^{\Delta t,+}))^\diamond, H_M(\rho_L^{\Delta t,+})) &= - \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty \int_\Omega \int_\Omega W_\tau(x, y) (\beta^L(\rho^{\Delta t,+})(x) \\
&\quad - \beta^L(\rho^{\Delta t,+})(y)) H_M(\rho^{\Delta t,+})(x)) dy dx \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau \\
&\quad + \frac{1}{\Gamma(-\alpha/2)} \int_0^\infty \int_\Omega \beta^L(\rho^{\Delta t,+})(y) H_M(\rho^{\Delta t,+})(y) (e^{-\tau \mathcal{L}_N} 1(y) - 1) dy \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau.
\end{aligned}$$

By summing the two expressions we then find that

$$\begin{aligned}
(\mathcal{L}_N^{\alpha/2}(\beta^L(\rho_L^{\Delta t,+}))^\diamond, H_M(\rho_L^{\Delta t,+})) &= - \frac{1}{2\Gamma(-\alpha/2)} \left(\iint\limits_{0 \leq \tau < \infty} \int_\Omega W_\tau(x, y) (\beta^L(\rho^{\Delta t,+})(x) - \beta^L(\rho^{\Delta t,+})(y)) \right. \\
&\quad \left. (H_M(\rho^{\Delta t,+})(x)) - H_M(\rho^{\Delta t,+})(y)) dx dy \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau \right. \\
&\quad \left. + 2 \iint\limits_{0 \leq \tau < \infty} \int_\Omega \beta^L(\rho^{\Delta t,+})(y) H_M(\rho^{\Delta t,+})(y) (1 - e^{-\tau \mathcal{L}_N} 1(y)) dy \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau \right). \tag{3.37}
\end{aligned}$$

Thanks to the definition of $\mathcal{L}_N$ stated and (3.4) we have that $e^{-\tau \mathcal{L}_N} 1(y) \leq 1$. Moreover the monotonicity of $\beta^L(\cdot)$ and $H_M(\cdot)$ ensure the positivity of both terms inside the outer brackets on the right-hand side of the above expression.

Thus, combining (3.35), (3.36) and (3.37), overall we have

$$\begin{aligned}
\int_0^{t_n} \int_{\Omega} \frac{\partial \rho_L^{\Delta t}}{\partial t} \zeta_M^{\epsilon}(\rho_L^{\Delta t,+}) dx dt &= - \int_0^{t_n} \int_{\Omega} (\zeta_M^{\epsilon})'(\rho_L^{\Delta t,+}) |\nabla \rho_L^{\Delta t,+}|^2 dx dt \\
&+ \frac{1}{2\Gamma(-\alpha/2)} \left(\int_0^{\infty} \int_{\Omega} \int_{\Omega} W_{\tau}(x, y) (\beta^L(\rho^{\Delta t,+})(x) - \beta^L(\rho^{\Delta t,+})(y)) (H_M(\rho^{\Delta t,+}(x)) \right. \\
&- H_M(\rho^{\Delta t,+}(y))) dx dy \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau \\
&\left. + \int_0^{\infty} \int_{\Omega} \beta^L(\rho^{\Delta t,+})(y) H_M(\rho^{\Delta t,+}(y)) (1 - e^{-\tau \mathcal{L}_N} 1(y)) dy \frac{1}{\tau^{1+\frac{\alpha}{2}}} d\tau \right). \quad (3.38)
\end{aligned}$$

All the terms in the above expression are nonpositive and therefore

$$\int_0^{t_n} \int_{\Omega} \frac{\partial \rho_L^{\Delta t}}{\partial t} \zeta_M^{\epsilon}(\rho_L^{\Delta t,+}) dx \leq 0 \quad (3.39)$$

Consider now the function $Z_M : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}$

$$Z_M(z) = \frac{1}{2} \max(z - M, 0)^2$$

and its regularisation $Z_M^{\epsilon} = Z_M * \theta_{\epsilon}$; the weak derivative of Z_M is clearly ζ_M and therefore, as before, we have $(Z_M^{\epsilon})'(z) = (Z_M' * \theta_{\epsilon})(z) = (\zeta_M * \theta_{\epsilon})(z)$; moreover notice that $\zeta_M^2 = 2Z_M$.

By performing the same computations as those in the proof of Lemma 1.16, with a Taylor expansion of $Z_M^{\epsilon}(\cdot)$, noting that $t \in [0, T] \mapsto \rho_L^{\Delta t}(\cdot, t)$ is piecewise affine relative to the temporal partition $0 = t_0 < t_1 < \dots < t_N = T$, we have that

$$\begin{aligned}
\int_0^{t_n} \int_{\Omega} \frac{\partial \rho_L^{\Delta t}}{\partial t} \zeta_M^{\epsilon}(\rho_L^{\Delta t,+}) dx d\tau &= \int_{\Omega} Z_M^{\epsilon}(\rho_L^{\Delta t,+}(x, t_n)) dx - \int_{\Omega} Z_M^{\epsilon}(\rho^0(x)) dx \\
&+ \frac{1}{2\Delta t} \int_0^{t_n} \int_{\Omega} (\zeta_M^{\epsilon})'(\theta_n \rho_L^{\Delta t,+} + (1 - \theta_n) \rho_L^{\Delta t,-}) (\rho_L^{\Delta t,+} - \rho_L^{\Delta t,-})^2 dx d\tau,
\end{aligned}$$

for $\theta_n \in (0, 1)$.

Thus, from (3.39) we directly have

$$\int_{\Omega} Z_M^{\epsilon}(\rho_L^{\Delta t,+}(x, t_n)) dx - \int_{\Omega} Z_M^{\epsilon}(\rho^0(x)) dx \leq 0.$$

If we set $M = \|\rho_0\|_{L^{\infty}(\Omega)}$, we have

$$\int_{\Omega} Z_{\|\rho_0\|_{L^{\infty}(\Omega)}}^{\epsilon}(\rho_L^{\Delta t,+}(x, t_n)) dx - \int_{\Omega} Z_{\|\rho_0\|_{L^{\infty}(\Omega)}}^{\epsilon}(\rho^0(x)) dx \leq 0.$$

Recalling that for any $M > 0$ we have $Z_M^{\epsilon} \rightarrow Z_M$ in $L^p([0, K])$, for any $K > 0$, $p \geq 1$, as $\epsilon \rightarrow 0$ (c.f. [50, Theorem 4.22]), if we send $\epsilon \rightarrow 0$,

$$\int_{\Omega} Z_{\|\rho_0\|_{L^{\infty}(\Omega)}}(\rho_L^{\Delta t,+}(x, t_n)) dx \leq \int_{\Omega} Z_{\|\rho_0\|_{L^{\infty}(\Omega)}}(\rho^0(x)) dx \leq \int_{\Omega} Z_{\|\rho_0\|_{L^{\infty}(\Omega)}}(\rho_0(x)) = 0$$

Using the fact that $Z_M \geq 0$ this then implies that

$$\int_{\Omega} Z_{\|\rho_0\|_{L^{\infty}(\Omega)}}(\rho_L^{\Delta t,+}(x, t_n)) dx = 0$$

Thus, we deduce that, for any $n = 1, \dots, N$, (3.34) must hold. $\square$

Therefore, we can drop immediately the upper cut-off parameter L in (3.33), by choosing $L > \|\rho_0\|_{L^\infty(\Omega)}$ and consider the problem

Find $\rho^{\Delta t}(\cdot, t) \in V = H^1(\Omega)$ for $t \in (0, T]$, such that

$$\int_0^T \int_\Omega \frac{\partial \rho^{\Delta t}}{\partial t} \phi \, dx = - \int_0^T \int_\Omega \nabla \rho^{\Delta t, +} \cdot \nabla \phi \, dx + \int_0^T \int_\Omega \rho^{\Delta t, +} A(x) \nabla c^{\Delta t, +} \cdot \nabla \phi \, dx \quad (3.40a)$$

$$\text{for all } \phi \in L^1(0, T; V), \quad (3.40b)$$

subject to the initial condition $\rho^{\Delta t}(x, 0) = \rho^0(x)$ for a.e. $x \in \Omega$, where $c_L^{\Delta t, +}(\cdot, t) \in \mathcal{H}_\diamond^1(\Omega)$ for all $t \in (0, T]$ and satisfies

$$-\mathcal{L}_N^s c^{\Delta t, +}(\cdot, t) = (\rho^{\Delta t, +})^\diamond(\cdot, t) \quad \text{in } \Omega,$$

for all $t \in (0, T]$.

We can now start to derive a bound that is uniform in Δt . Our candidate test function will be $\phi = \chi_{[0, t]} G'(\rho^{\Delta t, +})$, where $\chi_{[0, t]}$ denotes the characteristic function of the interval $[0, t]$. We recall that $r G''(r) = 1$ for all $r > 0$.

Thus, we take $\alpha \in (0, 1)$ and we choose $\phi = \chi_{[0, t]} G'(\rho^{\Delta t, +} + \alpha)$, with $t = t_n$, $n \in \{1, \dots, N\}$. We have

$$\begin{aligned} & \underbrace{\int_0^T \int_\Omega \frac{\partial \rho^{\Delta t}}{\partial t} \chi_{[0, t_n]} G'(\rho^{\Delta t, +} + \alpha) \, dx \, dt}_{\textcircled{1}} + \underbrace{\int_0^T \int_\Omega \nabla \rho^{\Delta t, +} \cdot \nabla \chi_{[0, t_n]} G'(\rho^{\Delta t, +} + \alpha) \, dx \, dt}_{\textcircled{2}} \\ & \quad = \underbrace{\int_0^T \int_\Omega \rho^{\Delta t, +} A(x) \nabla c^{\Delta t, +} \cdot \nabla \chi_{[0, t_n]} G'(\rho^{\Delta t, +} + \alpha) \, dx \, dt}_{\textcircled{3}}. \end{aligned}$$

Let us now manipulate the three terms one at a time. Terms $\textcircled{1}$ and $\textcircled{2}$ are treated as we did in the corresponding derivation in Section 1.3.

For the third term we have

$$\begin{aligned} \textcircled{3} &= \int_0^{t_n} \int_\Omega \rho^{\Delta t, +} G''(\rho^{\Delta t, +} + \alpha) A(x) \nabla c^{\Delta t, +} \cdot \nabla \rho^{\Delta t, +} \, dx \, d\tau \\ &= \int_0^{t_n} \int_\Omega \frac{\rho^{\Delta t, +}}{\rho^{\Delta t, +} + \alpha} A(x) \nabla c^{\Delta t, +} \cdot \nabla \rho^{\Delta t, +} \, dx \, d\tau. \end{aligned}$$

Putting everything together we therefore have that

$$\begin{aligned} & \int_\Omega G(\rho^{\Delta t, +}(x, t_n) + \alpha) \, dx + \frac{1}{2\Delta t (\|\rho_0\|_{L^\infty(\Omega)} + \alpha)} \int_0^{t_n} \int_\Omega (\rho^{\Delta t, +} - \rho^{\Delta t, -})^2 \, dx \, d\tau \\ & \quad + \int_0^{t_n} \int_\Omega \frac{|\nabla \rho^{\Delta t, +}|^2}{\rho^{\Delta t, +} + \alpha} \, dx \, d\tau \\ & \quad - \int_0^{t_n} \int_\Omega \frac{\rho^{\Delta t, +}}{\rho^{\Delta t, +} + \alpha} A(x) \nabla c^{\Delta t, +} \cdot \nabla \rho^{\Delta t, +} \, dx \, d\tau \\ & \leq \int_\Omega G(\rho^0(x) + \alpha) \, dx. \end{aligned}$$

We can now pass to the limit as $\alpha \rightarrow 0_+$ to obtain the following bound for $n = 1, \dots, N$, which is uniform in Δt thanks to (1.29):

$$\begin{aligned} & \int_{\Omega} G(\rho^{\Delta t,+}(x, t_n)) \, dx + \frac{1}{2\Delta t \|\rho_0\|_{L^\infty(\Omega)}} \int_0^{t_n} \int_{\Omega} (\rho^{\Delta t,+} - \rho^{\Delta t,-})^2 \, dx \, d\tau \\ & \quad + 4 \int_0^{t_n} \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t,+}} \right|^2 \, dx \, d\tau - \int_0^{t_n} \int_{\Omega} A(x) \nabla c^{\Delta t,+} \cdot \nabla \rho^{\Delta t,+} \, dx \, d\tau \\ & \leq \int_{\Omega} G(\rho^0(x)) \, dx \leq \int_{\Omega} G(\rho_0) \, dx. \end{aligned} \tag{3.41}$$

Finally we notice that

$$\int_{\Omega} A(x) \nabla c^{\Delta t,+}(x, t) \cdot \nabla \rho^{\Delta t,+}(x, t) \, dx = -(\mathcal{L}_N^{1-s}(\rho^{\Delta t,+})^\diamond, (\rho^{\Delta t,+})^\diamond).$$

Therefore, in case (K1), $Q = 0$ a.e. in Ω , the whole of the above expression is nonpositive and hence the term $-\int_{\Omega} A(x) \nabla c^{\Delta t,+}(x, t) \cdot \nabla \rho^{\Delta t,+}(x, t) \, dx$ in (3.41) can be discarded. Therefore, from (3.41), we have, for $n = 1, \dots, N$, that

$$\begin{aligned} & \int_{\Omega} G(\rho^{\Delta t,+}(x, t_n)) \, dx + \frac{1}{2\Delta t \|\rho_0\|_{L^\infty(\Omega)}} \int_0^{t_n} \int_{\Omega} (\rho^{\Delta t,+} - \rho^{\Delta t,-})^2 \, dx \, d\tau \\ & \quad + 4 \int_0^{t_n} \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t,+}} \right|^2 \, dx \, d\tau \\ & \leq \int_{\Omega} G(\rho_0) \, dx. \end{aligned} \tag{3.42}$$

Using property (1.29) we can supplement the above inequality with additional bounds, as we did in Section 1.3, and have

$$4 \int_0^T \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t,(\pm)}} \right|^2 \, dx \, dt \leq C_\star; \tag{3.43}$$

here and henceforth $C_\star$ stands for a generic positive constant, independent of Δt .

Notice that in this extended setting, obtaining a uniform bound on the norm of $c^{\Delta t,+}$ is not as straightforward as in Section 1.3. If we proceed as in Section 1.3, by choosing $-\chi_{[0,t_n]} c^{\Delta t,+}$ as a test function in (3.40a) and recalling (1.42) we have, for each $n \in \{1, \dots, N\}$, that

$$\begin{aligned} & - \int_0^{t_n} \int_{\Omega} \frac{\partial(\rho^{\Delta t})^\diamond}{\partial t} c^{\Delta t,+} \, dx \, d\tau \\ & \quad + \int_0^{t_n} \int_{\Omega} \rho^{\Delta t,+} A(x) \nabla c^{\Delta t,+} \cdot \nabla c^{\Delta t,+} \, dx \, d\tau = \int_0^{t_n} \int_{\Omega} \nabla \rho^{\Delta t,+} \cdot \nabla c^{\Delta t,+} \, dx \, d\tau, \end{aligned}$$

however the term on the right-hand side of the above expression no longer has a fixed sign and deriving a uniform bound on the norm of the potential $c^{\Delta t,+}$ is not achievable in this way. Nevertheless, the restriction on the fractional order $s \in (1/2, 1)$ and similar observations to the ones of Remark 3.9 can give us control on the gradient of $c^{\Delta t,+}$ in terms of the $L^2(0, T, L^2(\Omega))$

norm of $(\rho^{\Delta t,+})^\diamond$, which will allow us to perform the passage to the limit in Δt for the potential as well. In fact, we have

$$\begin{aligned}
\int_{\Omega} |\nabla c_L^{\Delta t,+}|^2 dx &\leq C(\mathcal{L}_N c_L^{\Delta t,+}, c_L^{\Delta t,+}) = C(\mathcal{L}_N^{1-s}(\rho_L^{\Delta t,+})^\diamond, \mathcal{L}_N^{-s}(\rho_L^{\Delta t,+})^\diamond) \\
&= C(\mathcal{L}_N^{1-2s}(\rho_L^{\Delta t,+})^\diamond, (\rho_L^{\Delta t,+})^\diamond) \\
&= C \sum_{k=1}^{\infty} \mu_k^{1-2s} ((\rho_L^{\Delta t,+})^\diamond)_k^2 \leq C \mu_1^{1-2s} \sum_{k=1}^{\infty} ((\rho_L^{\Delta t,+})^\diamond)_k^2 \\
&= C \mu_1^{1-2s} \|(\rho_L^{\Delta t,+})^\diamond\|_{L^2(\Omega)}^2.
\end{aligned} \tag{3.44}$$

We shall assume throughout the rest of the section that the test functions belong to the function space $L^2(0, T, W^{1,\infty}(\Omega))$. Our objective is, as in Chapter 1, to derive a (uniform in Δt) bound on the time-derivative of $\rho^{\Delta t}$ in terms of the $L^2(0, T, W^{1,\infty}(\Omega))$ norm of the test function, to apply Dubinskiĭ's compactness theorem. From (3.40a) we have that, for a test function $\phi \in L^2(0, T, W^{1,\infty}(\Omega))$,

$$\left| \int_0^T \int_{\Omega} \frac{\partial \rho^{\Delta t}}{\partial t} \phi dx dt \right| \leq \underbrace{\left| \int_0^T \int_{\Omega} \nabla \rho^{\Delta t,+} \cdot \nabla \phi dx dt \right|}_{\textcircled{1}} + \underbrace{\left| \int_0^T \int_{\Omega} \rho^{\Delta t,+} A(x) \nabla c^{\Delta t,+} \cdot \nabla \phi dx dt \right|}_{\textcircled{2}}.$$

We recall that we have

$$\begin{aligned}
\rho^{\Delta t,(\pm)} &\geq 0 \quad \text{a.e. on } \Omega \times (0, T), \quad \text{and} \\
\frac{1}{|\Omega|} \int_{\Omega} \rho^{\Delta t,(\pm)}(t) &= 1 \quad \text{for a.e. } t \in (0, T).
\end{aligned}$$

Moreover we notice that the bound on the first term on the left-hand side of (3.42) gives us a (uniform in Δt) bound on the $L^\infty(0, T; L^1(\Omega))$ norm of $\rho^{\Delta t,+}$, because the function $r \in [0, \infty) \mapsto G(r) \in [0, \infty)$ has superlinear growth as $r \rightarrow +\infty$.

The term $\textcircled{1}$ can be bound by $\left(\int_0^T \|\nabla \phi\|_{L^\infty(\Omega)}^2 dt \right)^{\frac{1}{2}}$, as we did in Section 1.3. For the term $\textcircled{2}$ we use the Cauchy-Schwarz inequality combined with (3.34), and the uniform ellipticity of $A(x)$ and (3.44), in order to get

$$\textcircled{2} \leq C_* \left(\int_0^T \|\nabla \phi\|_{L^\infty(\Omega)}^2 dt \right)^{\frac{1}{2}}.$$

By combining the bounds on the terms $\textcircled{1}$ and $\textcircled{2}$ and noting that by the Sobolev embedding theorem $H^{d+1}(\Omega)$ is continuously embedded in $W^{1,\infty}(\Omega)$ for $d = 2, 3$, we then have that

$$\left| \int_0^T \int_{\Omega} \frac{\partial \rho^{\Delta t}}{\partial t} \phi dx dt \right| \leq C_* \left(\int_0^T \|\nabla \phi\|_{L^\infty(\Omega)}^2 dt \right)^{\frac{1}{2}} \leq C_* \left(\int_0^T \|\phi\|_{H^{d+1}(\Omega)}^2 dt \right)^{\frac{1}{2}}. \tag{3.45}$$

We are now ready to take the limit as $\Delta t \rightarrow 0_+$. Our main tool to this end will still be Dubinskiĭ's compactness theorem in seminormed sets, that has been introduced in Chapter 1.

We collect the Δt -independent bounds (3.42), (3.43), (3.45) and the bound (3.44); we have shown that there exists a constant C_* , independent on Δt , such that

$$\begin{aligned} \sup_{t \in (0, T]} \int_{\Omega} G(\rho^{\Delta t, +}(t)) \, dx + \frac{1}{\Delta t} \int_0^T \int_{\Omega} (\rho^{\Delta t, +} - \rho^{\Delta t, -})^2 \, dx \, dt \\ + \int_0^T \int_{\Omega} \left| \nabla \sqrt{\rho^{\Delta t, (\pm)}} \right|^2 \, dx \, dt + \int_0^T \left\| \frac{\partial \rho^{\Delta t}}{\partial t} \right\|_{H^{-\beta}(\Omega)}^2 \, dt \leq C_*, \end{aligned} \quad (3.46)$$

$$\int_{\Omega} |\nabla c_L^{\Delta t, +}|^2 \leq C_* \|(\rho_L^{\Delta t, +})^{\diamond}\|_{L^2(\Omega)}^2. \quad (3.47)$$

Theorem 3.11. *Under the hypothesis that $Q = 0$ a.e. in Ω (case (K1)), there exists a subsequence of $\{\rho^{\Delta t, (\pm)}\}_{\Delta t > 0}$ (not indicated) and a function $\hat{\rho}$ such that*

$$\hat{\rho} \in L^{\infty}(0, T; L^{\infty}(\Omega)) \cap H^1(0, T; H^{-\beta}(\Omega)), \quad \beta = d + 1,$$

with $\hat{\rho} \geq 0$ almost everywhere on $\Omega \times (0, T)$ and $\frac{1}{|\Omega|} \int_{\Omega} \hat{\rho}(x, t) \, dx = 1$ for a.e. $t \in [0, T]$, and $\hat{c}(\cdot, t) \in \mathcal{H}_{\diamond}^s(\Omega) \cap H^1(\Omega)$ defined as $-\mathcal{L}_{\mathbf{N}}^s \hat{c}(\cdot, t) = \hat{\rho}^{\diamond}(\cdot, t)$ in Ω for $t \in (0, T]$ such that, for all $p \in [1, \infty)$,

$$\rho^{\Delta t, (\pm)} \rightarrow \hat{\rho} \quad \text{strongly in } L^p(0, T; L^1(\Omega)), \quad (3.48a)$$

$$\nabla \sqrt{\rho^{\Delta t, (\pm)}} \rightarrow \nabla \sqrt{\hat{\rho}} \quad \text{weakly in } L^2(0, T; L^2(\Omega; \mathbb{R}^d)), \quad (3.48b)$$

$$\frac{\partial \rho^{\Delta t}}{\partial t} \rightarrow \frac{\partial \hat{\rho}}{\partial t} \quad \text{weakly in } L^2(0, T; H^{-\beta}(\Omega)), \quad (3.48c)$$

$$\rho^{\Delta t, (\pm)} \rightarrow \hat{\rho} \quad \text{weakly-* in } L^{\infty}(0, T; L^{\infty}(\Omega)), \quad (3.48d)$$

$$\rho^{\Delta t, (\pm)} \rightarrow \hat{\rho} \quad \text{strongly in } L^p(0, T; L^p(\Omega)), \quad (3.48e)$$

$$c^{\Delta t, (\pm)} \rightarrow \hat{c} \quad \text{strongly in } L^p(0, T; \mathcal{H}^s(\Omega)), \quad (3.48f)$$

$$\nabla c^{\Delta t, +} \rightarrow \nabla \hat{c} \quad \text{weakly in } L^2(0, T; L^2(\Omega; \mathbb{R}^d)). \quad (3.48g)$$

The function $\hat{\rho}$ is a global weak solution to the problem

$$-\int_0^T \int_{\Omega} \hat{\rho} \frac{\partial \phi}{\partial t} \, dx \, dt + \int_0^T \int_{\Omega} \nabla \hat{\rho} \cdot \nabla \phi \, dx \, dt - \int_0^T \int_{\Omega} \hat{\rho} A(x) \nabla \hat{c} \cdot \nabla \phi \, dx \, dt = \int_{\Omega} \rho_0 \phi|_{t=0} \, dx \quad (3.48h)$$

for all $\phi \in W^{1,1}(0, T; H^{\beta}(\Omega))$ such that $\phi(\cdot, T) = 0$.

In addition, the function $\hat{\rho}$ is weak-* continuous as a mapping from $[0, T]$ to $L^{\infty}(\Omega)$ and it is weakly continuous as a mapping from $[0, T]$ to $L^1(\Omega)$.

Proof. The proofs for the convergence results (3.48a)-(3.48e) follow the same arguments as those used to prove (3.48a)-(3.48e) in Theorem 1.21, using the uniform bounds (3.46). Then, (3.48f) follows directly from (3.48e), (A.3) and (A.13c); that is,

$$\int_0^T \|c^{\Delta t, (\pm)}(t) - \hat{c}(t)\|_{\mathcal{H}_{\diamond}^s(\Omega)}^p \, dt \leq C \int_0^T \|\rho^{\Delta t, (\pm)}(t) - \hat{\rho}(t)\|_{L_{\diamond}^2(\Omega)}^p \, dt$$

for all $p \in [1, \infty)$.

Let us now consider the $L^2(0, T; L^2(\Omega; \mathbb{R}^d))$ norm of $\nabla c^{\Delta t, +}$. By the inequality (3.47) we have

$$\int_0^T \int_{\Omega} |\nabla c^{\Delta t, +}|^2 dx dt \leq C \int_0^T \int_{\Omega} ((\rho^{\Delta t, +})^\diamond)^2 dx dt$$

and thanks to the uniform bound on the $L^2(0, T; L^2(\Omega))$ norm of $\rho^{\Delta t, +}$ from the convergence (3.48e) we have that the $L^2(0, T; L^2(\Omega; \mathbb{R}^d))$ norm of the gradient of $c^{\Delta t, +}$ is uniformly bounded and therefore $\nabla c^{\Delta t, +}$ converges weakly to an element that we call H , as $\Delta t \rightarrow 0_+$. By (3.48f) with $s = 0$ we have that $\nabla c^{\Delta t, \pm}$ converges strongly to $\nabla \hat{c}$ in $L^2(0, T, H^{-1}(\Omega; \mathbb{R}^d))$, but then $\nabla \hat{c}$ must coincide with H because of the uniqueness of the weak limit.

We now want to use the convergence results we have just proved to pass to the limit as $\Delta t \rightarrow 0_+$ in equation (3.40). Throughout the argument we will consider test functions $\phi \in C^1([0, T]; C^\infty(\overline{\Omega}))$ such that $\phi(\cdot, T) = 0$. Note that the set of all such test functions is dense in the set of functions belonging to $W^{1,1}(0, T; H^\beta(\Omega))$ and vanishing at $t = T$ (in the sense of the trace theorem in $W^{1,1}(0, T)$), which is continuously embedded in $L^2(0, T; H^\beta(\Omega))$; therefore the use of such test functions is justified for the purposes of our argument.

For the first and second terms in (3.40a) we use the same procedure as in the proof of Theorem 1.21 to deduce that, as $\Delta t \rightarrow 0_+$,

$$\begin{aligned} \int_0^T \int_{\Omega} \frac{\partial \rho_L^{\Delta t}}{\partial t} \phi dx dt &\rightarrow - \int_0^T \int_{\Omega} \hat{\rho} \frac{\partial \phi}{\partial t} dx dt - \int_{\Omega} \rho_0 \phi|_{t=0} dx, \\ \lim_{\Delta t \rightarrow 0_+} \int_0^T \int_{\Omega} \nabla \rho^{\Delta t, +} \cdot \nabla \phi dx dt &= \int_0^T \int_{\Omega} \nabla \hat{\rho} \cdot \nabla \phi dx dt. \end{aligned}$$

Let us consider the final term in (3.40a). By (3.48g),

$$\nabla c^{\Delta t, +} \rightharpoonup \nabla \hat{c} \quad \text{weakly in } L^2(0, T; L^2(\Omega; \mathbb{R}^d))$$

and therefore $A(x) \nabla c^{\Delta t, +} \rightharpoonup A(x) \nabla \hat{c}$ weakly in $L^2(0, T; L^2(\Omega; \mathbb{R}^d))$, as $\Delta t \rightarrow 0_+$,

$$\begin{aligned} \int_0^T \int_{\Omega} A(x) \nabla c^{\Delta t, +} \cdot \nabla \phi dx dt &= \int_0^T \int_{\Omega} \nabla c^{\Delta t, +} \cdot A(x) \nabla \phi dx dt \\ &\rightarrow \int_0^T \int_{\Omega} \nabla \hat{c} \cdot A(x) \nabla \phi dx dt \\ &= \int_0^T \int_{\Omega} A(x) \nabla \hat{c} \cdot \nabla \phi dx dt, \end{aligned}$$

by the fact that if $\nabla \phi \in L^2(0, T, L^2(\Omega))$ then $A(x) \nabla \phi \in L^2(0, T, L^2(\Omega))$, thanks to A being bounded in $L^\infty(\Omega)$. Moreover, by (3.48e), $\rho^{\Delta t, +} \rightarrow \hat{\rho}$ strongly in $L^2(0, T; L^2(\Omega))$ and thus it follows that $\rho^{\Delta t, +} A(x) \nabla c^{\Delta t, +} \rightharpoonup \hat{\rho} A(x) \nabla \hat{c}$ weakly in $L^1(0, T; L^1(\Omega; \mathbb{R}^d))$. Therefore

$$\lim_{\Delta t \rightarrow 0_+} \int_0^T \int_{\Omega} \rho^{\Delta t, +} A(x) \nabla c^{\Delta t, +} \cdot \nabla \phi dx dt = \int_0^T \int_{\Omega} \hat{\rho} A(x) \nabla \hat{c} \cdot \nabla \phi dx dt$$

for all $\phi \in C^1([0, T]; C^\infty(\overline{\Omega}))$.

Putting these convergence results together, and noting that $C^1([0, T]; C^\infty(\overline{\Omega}))$ is dense in the function space $W^{1,1}(0, T; H^\beta(\Omega))$ with $\beta = d + 1$, we get (3.48h).

The proof of the weak-* continuity of the function $\widehat{\rho}$ as a map from $[0, T]$ to $L^\infty(\Omega)$ is identical to the proof of Theorem 1.21. $\square$

Remark 3.12. In conclusion, we highlight that the whole argument for passing to the limit $\Delta t \rightarrow 0_+$ has been possible through (3.34). If one could establish also in case (K0) (nonvanishing Q) a similar $L^\infty(\Omega)$ uniform control on the semidiscrete numerical approximations $\rho_L^{\Delta t, (\pm)}$ (up to a positive multiplicative constant, possibly depending on $\|Q\|_{L^\infty(\Omega)}$) this would yield an immediate extension of the previous proof of convergence as $\Delta t \rightarrow 0_+$. As noted previously, this fact, strongly suggested by numerical experiments, remains an open problem for future research.

Much as the draft turns into the sketch and the sketch into the painting through the serious work done on it, through the elaboration of the original vague idea and through the consolidation of the first fleeting and passing thought.

Vincent van Gogh (1853–1890), “Letter 133[F] July 1880”

4

Finite elements with weighted bases for the integral fractional Laplacian

In this chapter, we focus on the integral definition of the fractional Laplacian (4) that we have presented in the Introduction and the fractional Poisson equation, paired with a Dirichlet condition suitable for this definition, that is given by

$$\begin{cases} (-\Delta)^s u(x) = f(x), & x \in \Omega, \\ u(x) = 0, & x \in \mathbb{R}^d \setminus \Omega, \end{cases} \quad (4.1)$$

with Ω a bounded open subset of $\mathbb{R}^d$ and $f \in L^\infty(\Omega)$. We will refer to (4.1) as the *fractional Dirichlet problem*.

We recall that $a_s(\cdot, \cdot)$ is the bilinear form defined in (5) associated to the integral definition of the fractional Laplacian, the related fractional order Sobolev space $H^s(\mathbb{R}^d)$ is defined via (6), and the associated seminorm is $|w|_{H^s(\mathbb{R}^d)} := a_s(w, w)^{1/2}$. We point out that we have the following integration by parts formula

$$\int_{\mathbb{R}^d} \phi(x) (-\Delta)^s \psi(x) \, dx = a_s(\phi, \psi) \quad \text{for all } \phi, \psi \in C_0^\infty(\mathbb{R}^d).$$

In this and the following chapter, for ease of notation, we will denote by V the following space:

$$V := \{w \in H^s(\mathbb{R}^d) \text{ such that } w = 0 \text{ in } \mathbb{R}^d \setminus \Omega\}. \quad (4.2)$$

We also define the trace spaces for $s \in (0, 1)$ as $H_0^s(\Omega) := \overline{C_0^\infty(\Omega)}^{H^s}$. The fractional Poincaré inequality

$$\|u\|_{L^2(\Omega)} \leq C|u|_{H^s(\mathbb{R}^d)}, \quad \text{for all } u \in V, \quad (4.3)$$

(see [88]) ensures that the seminorm $|\cdot|_{H^s(\mathbb{R}^d)}$ is in fact an equivalent norm on V .

The problem (4.1) can then be written in weak form as follows:

$$\text{Find } u \in V \text{ such that } a_s(u, v) = \int_{\Omega} f(x)v(x) \, dx \quad \text{for all } v \in V. \quad (4.4)$$

The existence and uniqueness of a solution $u \in V$ to (4.4) is guaranteed by the coercivity and continuity of the bilinear form $a_s(\cdot, \cdot)$ and we refer to [5, Section 2] for a discussion on it.

Remark 4.1. We report two choices of the domain Ω and the right-hand side f for which an explicit solution to (4.1) is computable. The two examples are both insightful and they will be used in the numerical experiments of our method. In fact, the first example falls under our hypotheses for every $s \in (0, 1)$, while the second does not, but it still constitutes an interesting case to discuss.

When $\Omega = B_R(x_0)$ and $f = 1$, an explicit solution to (4.1) is given by

$$u^*(x) = c_{d,s} (R^2 - |x - x_0|^2)^s, \quad \text{where } c_{d,s} = \frac{\Gamma(d/2)}{2^{2s}\Gamma((d+2s)/2)\Gamma(1+s)}, \quad (4.5)$$

for $x \in \Omega$ (see [109, 36]).

On the unit ball, $\Omega = B_1$, the authors of [42], using Fourier transform techniques, computed the corresponding right-hand side of (4.1) when the solution u is $u(x) = (1 - |x|^2)_+$; this is given by

$$f(x) := (-\Delta)^s u(x) = \frac{4^s \Gamma(d/2 + s)}{\Gamma(d/2) \Gamma(2 - s)} {}_2F_1\left(\frac{d}{2} + s, s - 1; \frac{d}{2}; |x|^2\right), \quad (4.6)$$

where ${}_2F_1$ denotes the Gaussian hypergeometric function. We observe that, for $s \geq 1/2$ and $d = 1$, one has that $f \notin L^\infty(\Omega)$.

There are different reasons for which the integral fractional Laplacian and the Dirichlet problem (4.4) are more difficult to treat both from an analytical and numerical perspective than the spectral fractional Laplacian. The presence of a singular kernel in the definition (4) and in the corresponding bilinear form (5) constitutes the first challenge for any numerical approximation of it. Moreover, as we mentioned in the Introduction, there is a significant difference of regularity between the solution of a Dirichlet problem that is defined using the integral fractional Laplacian and the spectral fractional Laplacian: for the former the solution behaves like d_Ω^s in a neighbourhood of the boundary $\partial\Omega$, where $d_\Omega(x) = \text{dist}(x, \mathbb{R}^d \setminus \Omega)$, while for the latter the solution behaves simply as d_Ω . This substantial difference in regularity affects the convergence of finite element methods that have been developed for the problem (4.4). Important contributions [5, 4] that used piecewise linear basis functions on polygonal domains, report that convergence rates for these methods, in the s -fractional Sobolev-Slobodeckii norm, are at best approximately $h^{\frac{1}{2}}$, where h is the diameter of the mesh triangles. More precisely, under the additional assumptions that $f \in C^{\frac{1}{2}-s}(\Omega)$ if $0 < s < \frac{1}{2}$ and $f \in C^\beta(\Omega)$ for some $\beta \in (0, 2 - 2s)$

if $\frac{1}{2} < s < 1$, [5, Theorem 4.6] states that the piecewise linear finite element approximation u_h of the weak solution u to problem (4.1) satisfies the following estimate

$$|u - u_h|_{H^s(\mathbb{R}^d)} \leq \begin{cases} C h^{1/2} |\log h| \|f\|_{C^{\frac{1}{2}-s}(\overline{\Omega})}, & \text{if } s \in (0, 1/2), \\ C h^{1/2} |\log h| \|f\|_{L^\infty(\Omega)}, & \text{if } s = 1/2, \\ C h^{1/2} |\log h|^{1/2} \|f\|_{C^\beta(\overline{\Omega})}, & \text{if } s \in (1/2, 1), \end{cases} \quad (4.7)$$

where C stands for a positive constant. The sublinear convergence rates are due to the regularity of the solution u , which is at most $u \in H^{s+\frac{1}{2}-\varepsilon}(\Omega)$ for small $\varepsilon > 0$ because of its behaviour at the boundary (we refer the reader to [5, Proposition 3.6 and Proposition 3.11] and to [1] for a recent result of this type and [104, Section 2.7] for a summary of the related regularity results). The low regularity of u makes higher convergence rates difficult to obtain using a standard piecewise linear basis that is normally used for solutions that are at least once weakly differentiable. Furthermore, [5, Theorem 4.9] demonstrates that when graded meshes are employed, the convergence rate of approximately $h^{\frac{1}{2}}$ can be improved up to an almost linear rate, proportional to $N_h^{-\frac{1}{d}} |\log N_h^{-\frac{1}{d}}|^{1/2}$, for $s \in (1/2, 1)$, where N_h is the degrees of freedom (recall that in the case of uniform meshes $N_h \sim h^{-d}$). The study of H^1 rates is done in [45] for $s \in (1/2, 1)$ and, under additional assumptions on the right-hand side datum f , in the same paper the authors show for dimension $d = 1$ that graded meshes allow for H^s -rates of order h^{2-s} (see [45, Remark 4.5]). In [42] the authors improved the convergence rate to $h^{\kappa-s} |\log h|$ for $\kappa \in (s, 3/2)$, under the additional assumption that the solution to (4.1) possesses higher regularity at boundary. For example, when $u(x) = (1 - |x|^2)_+$ with $\Omega = B_1$ (the solution to (4.1) for f given by (4.6), see [42, Section 8.1]), the higher-order convergence rate $h^{\frac{3}{2}-s}$ in the s -fractional Sobolev–Slobodeckii norm can be achieved using piecewise linear basis functions. The assumption of [42] on the regularity of u , however, does not always hold for a general right-hand side $f \in L^\infty(\Omega)$. Recently, [101] established local interior error estimates of order up to h^{2-s} (see Corollary 2.4 therein), showing that the dominant errors associated with piecewise linear basis functions are indeed concentrated near the boundary. This observation further supports our approach, which is specifically designed to mitigate this primary source of error.

We also mention that hp -FEM has recently been applied to this problem. In [12, 102] the authors prove exponential convergence with respect to the number of degrees of freedom for hp -FEM, in $d = 1$ and $d = 2$ respectively. The implementation of hp -FEM for this problem is notoriously sophisticated because of several aspects, among which are the use of meshes with anisotropic geometric refinement towards the boundary and an exponentially accurate quadrature rule for the bilinear form $a_s(\cdot, \cdot)$; in [13] the authors provide an implementation for the one-dimensional setting.

The method that we present in this chapter builds on the observation that, intuitively, if δ denotes a smooth approximation of the distance function d_Ω , then the quotient u/δ^s exhibits

significantly better regularity up to the boundary, provided that both f and the domain Ω are sufficiently smooth. This regularity theory has been developed through a series of contributions [152, 114, 155, 156, 157, 1, 3]. The example (4.5) in Remark 4.1 well illustrates the high regularity of u/d_Ω^s . Motivated by this fact, we construct a tailored finite element basis that captures the improved regularity of u/δ^s , thereby achieving higher-order convergence rates than those available in the existing literature. The idea is to use a basis of the form $\delta^s \times$ (piecewise linear functions). In fact, one of the key advantages of the finite element method is its effectiveness in approximating smooth functions and our method takes advantage of this well-known fact in order to approximate u/δ^s and subsequently, knowing δ^s , the solution u itself. This consideration motivates our strategy of approximating u/δ^s rather than u directly.

We mention that specialised finite element bases have been employed in other contexts, such as acoustic and electromagnetic scattering, to mitigate the growth in the number of degrees of freedom required by standard finite element methods to maintain a given accuracy. We refer the reader to [68, 69], where products of piecewise polynomials with plane waves were chosen, or to [113], for oscillatory basis functions capturing the high-frequency solution behaviour in a transmission problem.

The advantage of this approach is that we can obtain improved convergence rates, without requiring higher regularity of u , but rather assuming that f and Ω are sufficiently smooth, which is sometimes the case in applications. Assuming sufficient regularity of the right-hand side f and the domain Ω , we obtain convergence rates of order $h^{2-s}|\log h|^{\frac{1}{2}}$ in the s -fractional Sobolev-Slobodeckii norm for $s \in (0, 1)$, improving all previously reported results in the literature. Using Aubin-Nitsche duality, we also obtain L^2 -rates of higher order than our H^s -rates.

4.1 Generic regularity of the solution to the fractional Dirichlet problem

For $\alpha > 0$ let us denote by $W^{\alpha,\infty}(\Omega)$ the Hölder space of order α

$$W^{\alpha,\infty}(\Omega) := C^{[\alpha]-1, \alpha-[\alpha]+1}(\overline{\Omega}).$$

We recall that Morrey's inequality guarantees that for all $\alpha > 0$ we have $H^{\alpha+\frac{d}{2}}(\mathbb{R}^d) \subset W_{\text{loc}}^{\alpha,\infty}(\mathbb{R}^d)$ (cf. [133, Theorem 7.23] for example).

We now present the regularity theory for the solution of problem (4.1), that we will use for the design of our finite element method.

Given the distance function $d_\Omega(x) = \text{dist}(x, \mathbb{R}^d \setminus \Omega)$ for $x \in \mathbb{R}^d$, we consider modified distance functions δ satisfying for some $c, c_\alpha > 0$:

$$\begin{aligned} \delta \in C^\infty(\Omega) \cap W^{\sigma,\infty}(\Omega) \text{ with } \frac{1}{c}d_\Omega \leq \delta \leq c d_\Omega \text{ in } \mathbb{R}^d \text{ and} \\ \left| \left(\frac{\partial}{\partial x} \right)^\alpha \delta \right| \leq c_\alpha \delta^{\sigma-|\alpha|} \text{ in } \Omega \text{ for all multi-indices } \alpha \text{ with } |\alpha| > \sigma. \end{aligned} \quad (4.8)$$

By its definition, d_Ω vanishes identically on $\mathbb{R}^d \setminus \Omega$, and the two-sided bound $\frac{1}{c}d_\Omega \leq \delta \leq c d_\Omega$ in (4.8) forces $\delta \equiv 0$ outside of Ω . Accordingly, we always understand δ to be extended by zero outside of Ω , and the smoothness imposed in (4.8), and used in the regularity results below, is interior only.

Remark 4.2. The existence of a function δ satisfying (4.8) can be ensured under regularity assumptions on the domain Ω . More precisely, a natural choice in general domains can be found in [1, Lemma A.2] under the assumption $\sigma > 1$ and $\sigma \notin \mathbb{N}$ and $\partial\Omega \in C^{k,t}$ with $k \in \mathbb{N}$, $t \in (0, 1)$ and $k + t = \sigma$; with these hypotheses the function δ is shown to be the solution of

$$\begin{cases} -\Delta\delta(x) = 1, & x \in \Omega, \\ \delta(x) = 0, & x \in \partial\Omega. \end{cases} \quad (4.9)$$

In some scenarios, there are simpler ways of obtaining a suitable function δ rather than solving (4.9). For example, if $\Omega = B_R(x_0)$, we can choose $\delta(x) = R^2 - |x - x_0|^2$ or $\delta(x) = R^4 - |x - x_0|^4$. We anticipate that we will often take the latter for the numerical experiments.

We recall that a domain Ω satisfies the exterior ball condition if there exists a positive radius such that, at every point of $\partial\Omega$, there is an exterior ball of that radius tangent to $\partial\Omega$ at that point. Using super-solution arguments, it was shown (see [152, Lemma 2.7]) that, for a bounded domain Ω satisfying the exterior ball condition, the solution u of problem (4.1) satisfies the following estimate:

$$|u(x)| \leq C \|f\|_{L^\infty(\Omega)} d_\Omega(x)^s, \quad \text{for all } f \in L^\infty(\Omega). \quad (4.10)$$

Moreover, explicit estimates for the Green kernel (see [72]) yield

$$u(x) \geq c d_\Omega(x)^s \int_\Omega f(y) d_\Omega(y)^s dy, \quad \text{for all } f \geq 0. \quad (4.11)$$

Thus, u behaves like d_Ω^s for nonnegative and bounded f . In [152], it was proved that if $f \in C^\alpha(\overline{\Omega})$ with small $\alpha > 0$, then $u/d_\Omega^s \in C^{\alpha+s}(\overline{\Omega})$. Similar result for arbitrary $\alpha > 0$ was later established. In particular, [1, Theorems 1.3 and 1.4] proved the following higher regularity result, valid for a regularised distance δ satisfying (4.8) with $\sigma = \gamma + 1$:

$$\partial\Omega \in C^{\gamma+1}, f \in C^{(\gamma-s)+}(\overline{\Omega}) \implies \frac{u}{\delta^s} \in W^{\gamma,\infty}(\Omega), \quad \text{for all } \gamma > 0 \text{ such that } \gamma, \gamma \pm s \notin \mathbb{N}. \quad (4.12)$$

We also mention [114, 3] where it is proved that if $\Omega \in C^\infty$ and $\delta, f \in C^\infty(\overline{\Omega})$ then $u/\delta^s \in C^\infty(\overline{\Omega})$.

4.2 Weighted finite element method

We now introduce the notation and the construction of our finite element method for the fractional Dirichlet problem. As (4.12) shows, our approach will rely on the regularity of the domain

Ω , however standard finite element methods are usually based on polygonal or polyhedral domains, no more regular than Lipschitz. We circumvent this problem by defining a triangulation that mesh a slightly larger domain Ω_h .

Given a domain Ω , let us consider a sequence $(\mathcal{T}_h)_{h>0}$ where each $\mathcal{T}_h$ is a set of simplices (i.e., intervals if $d = 1$, triangles if $d = 2$, and tetrahedra if $d = 3$) that satisfies the following properties:

- $\bar{\Omega} \subset \bigcup_{K \in \mathcal{T}_h} \bar{K}$ and for $K \in \mathcal{T}_h$ we have $\bar{K} \cap \bar{\Omega} \neq \emptyset$; we define

$$\Omega_h := \left(\bigcup_{K \in \mathcal{T}_h} \bar{K} \right)^\circ,$$

namely the interior of the union of the closures of all simplices;

- for $K \in \mathcal{T}_h$, we denote by $h_K := \text{diam}(K)$ and ξ_K the diameter of the largest sphere inscribed in K . We assume that there exists a constant $c > 0$ such that $\max_{K \in \mathcal{T}_h} \frac{h_K}{\xi_K} \leq c$; in this case, we say that the triangulation is *shape regular*;
- there are constants $c_1, c_2 > 0$ and there exists $h > 0$, such that $c_1 h \leq h_K \leq c_2 h$ for any $K \in \mathcal{T}_h$; we say that the triangulation is *quasi-uniform*;
- any face of any simplex $K \in \mathcal{T}_h$ is either a subset of the boundary $\partial\Omega_h$ or a face of another simplex; we say that such a triangulation is *conforming*.

We call this set of simplices an “*over-triangulation*” of Ω . Given an over-triangulation $\mathcal{T}_h$ we define

$$\text{PL}(\mathcal{T}_h) := \{v_h \in C(\bar{\Omega}_h) \text{ such that } v_h|_K \in \mathbb{P}^1 \text{ for all } K \in \mathcal{T}_h\}.$$

We notice that, when $d > 1$, if Ω is regular then $\Omega \subsetneq \Omega_h$, see Figure 4.1. Let us also introduce the notation

$$\delta^s \text{PL}(\mathcal{T}_h) := \{\delta^s v_h : v_h \in \text{PL}(\mathcal{T}_h)\}.$$

The multiplication by δ^s disregards any information outside Ω (we recall that $d_\Omega(x) = \text{dist}(x, \mathbb{R}^d \setminus \Omega)$); this is a reason for which it is technically convenient to over-mesh the domain.

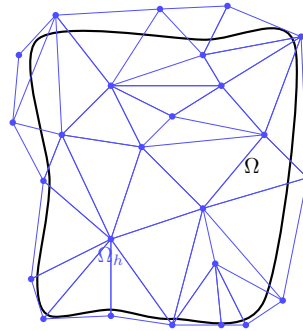


Figure 4.1: Example of over-triangulation.

We want to set up a finite element method for problem (4.4). Given a regularisation δ of the distance to the boundary function d_Ω (see (4.8)), and an over-triangulation $\mathcal{T}_h$, we consider the finite-dimensional subspace of $H_0^s(\Omega)$ given by

$$V_h := \{v : \mathbb{R}^d \rightarrow \mathbb{R} \text{ such that } v|_\Omega \in \delta^s \text{PL}(\mathcal{T}_h) \text{ and } v = 0 \text{ in } \mathbb{R}^d \setminus \Omega\}. \quad (4.13)$$

Let us also define $N_h := \dim V_h$. We denote by $\{P_j\}_{j=1}^{N_h}$ the vertices of all simplexes $K \in \mathcal{T}_h$ (including those lying in $\partial\Omega_h$). Therefore, the canonical basis of $\text{PL}(\mathcal{T}_h)$ is given by the piecewise linear functions ϕ_i such that $\phi_i(P_j) = \delta_{ij}$. Then, the canonical basis of the space V_h is made of the functions $\zeta_i = \delta^s \phi_i$. When we use the basis $\{\zeta_i\}_{i=1}^{N_h}$, we will refer to the resulting numerical method as the weighted finite element method, or WFEM for short. Notice u/δ^s may not vanish on $\partial\Omega$, so we need to include the nodes $P_i \in \partial\Omega_h$.

The most common FEM approach for the Dirichlet problem is considered on exactly-meshable domains $\Omega = \Omega_h$ (see, e.g., [5]). In that case $\partial\Omega$ is no better than Lipschitz, and can be expressed in terms of our notation as $\Omega = \Omega_h$. In this case, the standard approximation space is $V_h^{\text{FEM}} := \text{PL}(\mathcal{T}_h) \cap W_0^{1,\infty}(\Omega)$ and the canonical basis of this space is $\{\phi_i : P_i \in \Omega\}$.

In order to highlight this difference, we discuss the case $\Omega = (-1, 1)$, and consider $h > 0$. We denote the points $P_i = -1 + (i-1)h$ for $i = 1, \dots, N_h$. We can write the basis for standard FEM for the Dirichlet problem as

$$V_h^{\text{FEM}} = \text{span}\{\phi_2, \dots, \phi_{N_h-1}\}.$$

The WFEM approximation space is

$$V_h = \text{span}\{\delta^s \phi_1, \dots, \delta^s \phi_{N_h}\}.$$

We show the comparison between the two bases in Figure 4.2. In order to handle homogeneous Dirichlet boundary conditions in the standard FEM, the piecewise linear functions centered at points located outside the interior of the domain Ω are not included in the basis. In contrast, for WFEM, these functions are also part of the basis. Heuristically, this can be understood by noting that the approximation is performed on the quantity u/δ^s , which, in general, does not vanish on the boundary $\partial\Omega$. In this sense, the basis used in the WFEM for the homogeneous Dirichlet case can be obtained by multiplying by δ^s a basis that would correspond to the Neumann case in the standard FEM. For this reason, in Figure 4.2, we depict some basis functions for WFEM corresponding to different functions δ and we compare them to the standard FEM basis functions in case of a Dirichlet and Neumann boundary conditions.

With this notation, we define the associated finite element approximation problem as follows:

$$\text{Find } u_h \in V_h \text{ such that } a_s(u_h, v_h) = \int_\Omega f(x) v_h(x) dx \quad \text{for all } v_h \in V_h. \quad (4.14)$$

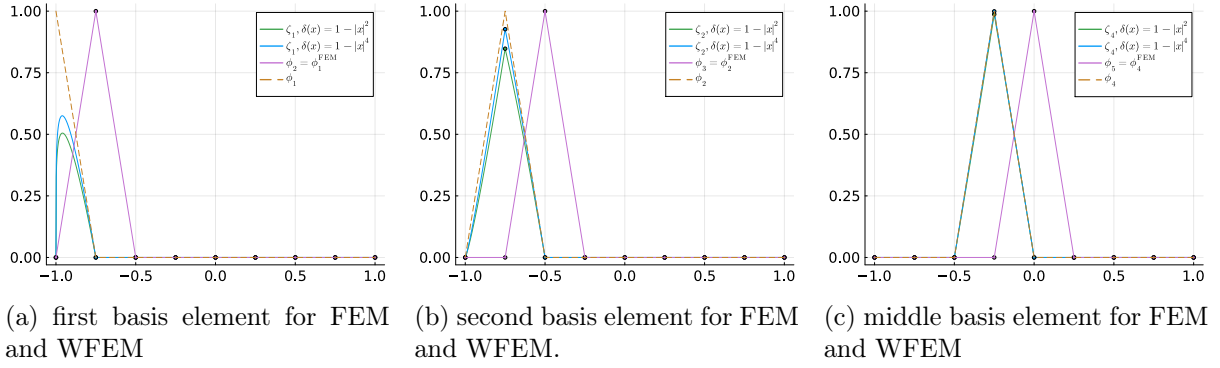


Figure 4.2: FEM and WFEM basis function on $\Omega = (-1, 1)$ for $s = 0.2$ and $h = 0.25$

Since the bilinear form $a_s(\cdot, \cdot)$ is coercive, applying the Lax-Milgram theorem yields well-posedness of (4.14). In practice, if $\{\zeta_i\}_{i=1}^{N_h}$ is a basis for V_h problem (4.14) is equivalent to

$$\text{Find } u_h \in V_h \text{ such that } a_s(u_h, \zeta_i) = \int_{\Omega} f(x) \zeta_i(x) dx \quad \text{for all } i = 1, \dots, N_h. \quad (4.15)$$

Since $u_h \in V_h$, one can write $u_h = \sum_{i=1}^{N_h} U_i \zeta_i$ and then (4.15) is equivalent to computing the vector U , solution of the linear system

$$A_s U = F, \quad A_s \in \mathbb{R}^{N_h \times N_h}, \quad (A_s)_{i,j} = a_s(\zeta_j, \zeta_i), \quad F \in \mathbb{R}^{N_h}, \quad F_i = (f, \zeta_i). \quad (4.16)$$

We remark that for WFEM the rows and columns of A_s corresponding to nodes lying outside Ω contain only zeros. At the level of implementation, these rows and columns, together with the corresponding entries of the load vector F , are therefore removed before (4.16) is solved.

4.3 Convergence results

We present in this section the convergence rate in h of the numerical method (4.14) based on weighted elements.

In order to prove some of our results, we need to extend Hölder functions from Ω to Ω_h and $\mathbb{R}^d$. To this end, let B_R be a ball such that

$$\overline{\Omega} \subset \overline{\Omega_h} \subset B_R.$$

Let Ω be such that $\partial\Omega \in C^{1,1}$. For any $\mu \in (0, 2]$ consider a linear extension operator E_μ satisfying

$$\begin{aligned} E_\mu : W^{\mu,\infty}(\overline{\Omega}) &\rightarrow W^{\mu,\infty}(\mathbb{R}^d), \quad E_\mu u = u \text{ in } \Omega, \quad \text{supp}\{E_\mu u\} \subset B_R, \\ \|E_\mu u\|_{W^{\mu,\infty}(\mathbb{R}^d)} &\leq C \|u\|_{W^{\mu,\infty}(\overline{\Omega})}, \quad \text{for some constant } C = C(d, \mu, \Omega, R). \end{aligned} \quad (4.17)$$

The existence of such an extension operator can be found in [166, Chapter VI, Theorem 3] and [111, Lemma 6.37]. We point out that in the construction of [166] $E_\mu = E_1$ for all $\mu \in (0, 1]$.

Furthermore, $E_1 : C(\overline{\Omega}) \rightarrow C_b(\mathbb{R}^d)$. Lastly, let us introduce the restriction r_Ω such that $r_\Omega u = u|_\Omega$.

The following fact will be needed for the convergence results.

Lemma 4.3. *Let $s \in (0, 1)$, $\partial\Omega \in C^{1,1}$ and δ satisfy (4.8) with $\sigma = 1$. Then $V_h \subset V$.*

Proof. Let $v \in V_h$. By definition $v = 0$ in $\mathbb{R}^d \setminus \Omega$. Let us now check that $v \in H^s(\mathbb{R}^d)$. Clearly,

$$\|v\|_{L^2(\mathbb{R}^d)} = \|v\|_{L^2(\Omega)} \leq |\Omega|^{\frac{1}{2}} \|v\|_{L^\infty(\mathbb{R}^d)}.$$

On the other hand, we can write $v = \delta^s E_1 r_\Omega w$ for some $w \in \text{PL}(\mathcal{T}_h) \subset W^{1,\infty}(\Omega_h)$. Thus,

$$\begin{aligned} |v|_{H^s(\mathbb{R}^d)} &= |\delta^s E_1 w|_{H^s(\mathbb{R}^d)} \\ &\leq \|\delta^s\|_{L^\infty(\mathbb{R}^d)} |E_1 w|_{H^s(\mathbb{R}^d)} + |\delta^s|_{H^s(\mathbb{R}^d)} \|E_1 w\|_{L^\infty(\mathbb{R}^d)} \end{aligned}$$

Clearly $\|\delta^s\|_{L^\infty(\mathbb{R}^d)}, \|E_1 w\|_{L^\infty(\mathbb{R}^d)} < +\infty$ and due to Lemma B.1 we have $|\delta^s|_{H^s(\mathbb{R}^d)} < \infty$. Finally, we note that, by the properties of the extension operator E_1 and the standard interpolation inequality (see [137]), we have that

$$\|E_1 w\|_{H^s(\mathbb{R}^d)} \leq C(s) \|E_1 w\|_{L^2(\mathbb{R}^d)}^{1-s} \|E_1 w\|_{H^1(\mathbb{R}^d)}^s \leq C(s, R) \|E_1 w\|_{L^2(\mathbb{R}^d)}^{1-s} \|E_1 w\|_{W^{1,\infty}(\mathbb{R}^d)}^s < +\infty,$$

where $C(s), C(s, R)$ are positive constants and R is the constant in (4.17). $\square$

As usual in the finite elements setting, we rely on the following Céa's lemma to prove the desired convergence result.

Lemma 4.4 (Céa's lemma). *Let $s \in (0, 1)$, $\partial\Omega \in C^{1,1}$ and δ satisfy (4.8) with $\sigma = 1$. Let also u be the corresponding solution of (4.4), let V_h be given by (4.13), and let u_h be the solution of (4.14). Then,*

$$|u - u_h|_{H^s(\mathbb{R}^d)} = \min_{v_h \in V_h} |u - v_h|_{H^s(\mathbb{R}^d)}. \quad (4.18)$$

Proof. We recall that $V_h \subset V$ as shown in Lemma 4.3. The inequality $\geq$ in (4.18) holds because $u_h \in V_h$. Let $v_h \in V_h$. For any $w_h \in V_h$ we can use the weak formulation to deduce that $a_s(u - u_h, w_h) = a_s(u, w_h) - a_s(u_h, w_h) = \int_\Omega f w_h - \int_\Omega f w_h = 0$. Therefore, we have that

$$\begin{aligned} |u - u_h|_{H^s(\mathbb{R}^d)}^2 &= a_s(u - u_h, u - u_h) = a_s(u - u_h, u) \\ &= a_s(u - u_h, u) - a_s(u - u_h, v_h) = a_s(u - u_h, u - v_h). \end{aligned}$$

Using the Cauchy-Schwarz inequality we have that

$$|u - u_h|_{H^s(\mathbb{R}^d)}^2 \leq |u - u_h|_{H^s(\mathbb{R}^d)} |u - v_h|_{H^s(\mathbb{R}^d)}.$$

If $|u - u_h|_{H^s(\mathbb{R}^d)} = 0$ then (4.18) holds trivially because $|\cdot|_{H^s(\mathbb{R}^d)} \geq 0$. If $|u - u_h|_{H^s(\mathbb{R}^d)} > 0$ then we can divide by $|u - u_h|_{H^s(\mathbb{R}^d)}$ to prove the $\leq$ part of (4.18). $\square$

In order to build a suitable competitor to apply C  a's Lemma and obtain the desired orders of convergence, we need to define a suitable interpolant. More precisely, let $I_h : C(\mathbb{R}^d) \rightarrow \text{PL}(\mathcal{T}_h) \subset W^{1,\infty}(\Omega_h)$ be the piecewise linear interpolation obtained by sampling at the vertices of the simplices in $\mathcal{T}_h$. We define, for $\mu \in (s, 2]$, the map $J_h : \delta^s W^{\mu,\infty}(\mathbb{R}^d) \rightarrow V_h$ by

$$J_h v := \delta^s E_1 r_\Omega I_h E_\mu \frac{v}{\delta^s}. \quad (4.19)$$

We do not include the dependence on μ in the definition of J_h for the sake of clarity. Notice that since $E_\alpha w = w$ in Ω for any α , for any $\alpha > 0$ we have that

$$J_h v = \delta^s E_\alpha r_\Omega I_h E_\mu \frac{v}{\delta^s}.$$

The aim of $J_h v$ is to give a correct meaning to $\delta^s I_h \frac{v}{\delta^s}$, where v/δ^s is only defined in Ω but not in Ω_h .

We now show that the interpolation operator I_h is bounded in $W^{\alpha,\infty}$ for $\alpha \in (0, 1]$.

Lemma 4.5. *Let $w \in W^{\alpha,\infty}(\mathbb{R}^d)$ for $\alpha \in (0, 1]$. Then,*

$$\|I_h w\|_{W^{\alpha,\infty}(\Omega)} \leq C \|w\|_{W^{\alpha,\infty}(\mathbb{R}^d)},$$

where C depends only on α , Ω , and the mesh regularity constant of $\mathcal{T}_h$.

Proof. First, assume that $w \in W^{1,\infty}(\mathbb{R}^d)$. A trivial computation yields that, for all $\phi \in W^{1,\infty}(\mathbb{R}^d)$,

$$\|I_h \phi\|_{L^\infty(\Omega_h)} \leq \max_{\Omega_h} |\phi|, \quad \|\nabla I_h \phi\|_{L^\infty(\Omega_h)} \leq C \max_{\Omega_h} |\nabla \phi|, \quad (4.20)$$

where C stands for a positive constant that does not depend on h . We observe that the operator $T_h = E_1 \circ r_\Omega \circ I_h$ is

$$T_h : C_b(\mathbb{R}^d) \rightarrow L^\infty(\mathbb{R}^d), \quad T_h : C_b^1(\mathbb{R}^d) \rightarrow W^{1,\infty}(\mathbb{R}^d).$$

Applying the K -method of function space interpolation [137, Theorem 1.6, Example 1.8, and the result after proof Example 1.8] with $T_h : W^{\alpha,\infty}(\mathbb{R}^d) \rightarrow W^{\alpha,\infty}(\mathbb{R}^d)$, we have

$$\|T_h\|_{\mathcal{L}(W^{\alpha,\infty}(\mathbb{R}^d), W^{\alpha,\infty}(\mathbb{R}^d))} \leq C(\alpha, d) \|T_h\|_{\mathcal{L}(C_b(\mathbb{R}^d), L^\infty(\mathbb{R}^d))}^{1-\alpha} \|T_h\|_{\mathcal{L}(C_b^1(\mathbb{R}^d), W^{1,\infty}(\mathbb{R}^d))}^\alpha,$$

where $\mathcal{L}(X, Y)$ denotes the space of all linear bounded operators from X to Y and $C(\alpha, d)$ is a positive constant depending only on α and d . The right-hand side of the above inequality can be then bounded independently on h by (4.20). Therefore, we can write

$$\|I_h w\|_{W^{\alpha,\infty}(\Omega)} \leq \|E_1 r_\Omega I_h w\|_{W^{\alpha,\infty}(\mathbb{R}^d)} = \|T_h w\|_{W^{\alpha,\infty}(\mathbb{R}^d)} \leq C \|w\|_{W^{\alpha,\infty}(\mathbb{R}^d)}. \quad \square$$

Thus, we can derive a $W^{\alpha,\infty}$ norm convergence rate for the interpolation operator I_h .

Lemma 4.6. For $\alpha \in (0, 1]$ and $\mu \in (\alpha, 2]$ we have that, for all $w \in W^{\mu, \infty}(\mathbb{R}^d)$,

$$\|w - I_h w\|_{W^{\alpha, \infty}(\Omega)} \leq Ch^{\mu-\alpha} \|w\|_{W^{\mu, \infty}(\mathbb{R}^d)},$$

where C depends only on α, μ, Ω , and the mesh regularity constants of the triangulation.

Proof. First, for $w \in W^{2, \infty}(\mathbb{R}^d)$, we apply [74, Theorem 3.1.5], estimating interpolation error on every element and then passing from local interpolation error to global interpolation error, to show the result for integer values α, μ , i.e.,

$$\|w - I_h w\|_{L^\infty(\Omega_h)} \leq Ch^2 \|w\|_{W^{2, \infty}(\Omega_h)}, \quad \|w - I_h w\|_{W^{1, \infty}(\Omega_h)} \leq Ch \|w\|_{W^{2, \infty}(\Omega_h)},$$

where C depends only on the mesh regularity constants of the triangulation. Let $\eta \in C_0^\infty(\mathbb{R}^d)$ with support B_1 . We take $\eta_\epsilon(x) = \epsilon^{-d} \eta(x/\epsilon)$. Let $w_\epsilon = \eta_\epsilon * w$. We have the estimates

$$\|w_\epsilon\|_{W^{2, \infty}(\mathbb{R}^d)} \leq C_\eta \epsilon^{\mu-2} \|w\|_{W^{\mu, \infty}(\mathbb{R}^d)}, \quad \|w - w_\epsilon\|_{W^{\alpha, \infty}(\mathbb{R}^d)} \leq C_\eta \epsilon^{\mu-\alpha} \|w\|_{W^{\mu, \infty}(\mathbb{R}^d)}, \quad (4.21)$$

for a positive constant $C_\eta > 0$. Now we observe that for $\alpha \in (0, 1]$ we have

$$\begin{aligned} |u|_{W^{\alpha, \infty}(\Omega_h)} &= \sup_{\substack{x, y \in \Omega_h \\ x \neq y}} \frac{|u(x) - u(y)|}{|x - y|^\alpha} = \sup_{\substack{x, y \in \Omega_h \\ x \neq y}} |u(x) - u(y)|^{1-\alpha} \left(\frac{|u(x) - u(y)|}{|x - y|} \right)^\alpha \\ &\leq 2^{1-\alpha} \|u\|_{L^\infty(\Omega_h)}^{1-\alpha} |u|_{W^{1, \infty}(\Omega_h)}^\alpha. \end{aligned} \quad (4.22)$$

Now we can use interpolation, applying (4.22), to deduce that, for $\alpha \in (0, 1]$,

$$|w - I_h w|_{W^{\alpha, \infty}(\Omega_h)} \leq Ch^{2-\alpha} \|w\|_{W^{2, \infty}(\Omega_h)}. \quad (4.23)$$

As a last step, we interpolate on the right-hand side by using convolutions recalling the rates (4.21). We can write using Lemma 4.5 that

$$\begin{aligned} |w - I_h w|_{W^{\alpha, \infty}(\Omega)} &\leq |w - w_\epsilon|_{W^{\alpha, \infty}(\Omega)} + |w_\epsilon - I_h w_\epsilon|_{W^{\alpha, \infty}(\Omega)} + |I_h w_\epsilon - I_h w|_{W^{\alpha, \infty}(\Omega)} \\ &\leq C |w - w_\epsilon|_{W^{\alpha, \infty}(\Omega)} + |w_\epsilon - I_h w_\epsilon|_{W^{\alpha, \infty}(\Omega)}. \end{aligned}$$

The first term on the right-hand side of the above expression can be controlled using (4.21) by $C\epsilon^{\mu-\alpha} \|w\|_{W^{\mu, \infty}(\mathbb{R}^d)}$. We estimate the other term also using (4.21) together with (4.23):

$$|w_\epsilon - I_h w_\epsilon|_{W^{\alpha, \infty}(\Omega)} \leq h^{2-\alpha} \|w_\epsilon\|_{W^{2, \infty}(\Omega_h)} \leq h^{2-\alpha} \epsilon^{\mu-2} \|w\|_{W^{\mu, \infty}(\mathbb{R}^d)}.$$

Taking $\epsilon = h$ completes the proof. $\square$

We prove now the order of approximation of a suitable competitor.

Lemma 4.7. Let $s \in (0, 1)$, $\partial\Omega \in C^{1,1}$, $\mu \in (s, 2]$, and let δ satisfy (4.8) with $\sigma = \max\{1, \mu\}$. Let also $v \in \delta^s C(\bar{\Omega})$ such that $v/\delta^s \in W^{\mu,\infty}(\bar{\Omega})$. Then, for all $\alpha \in (s, \min\{\mu, 1\}]$, we have that

$$|v - J_h v|_{H^s(\mathbb{R}^d)} \leq \frac{C_1}{\sqrt{\alpha - s}} h^{\mu-\alpha} \|v/\delta^s\|_{W^{\mu,\infty}(\Omega)}, \quad (4.24)$$

with $C_1 = C_1(\Omega, d, s, \mu) > 0$. In particular, we have that

$$|v - J_h v|_{H^s(\mathbb{R}^d)} \leq C_2 h^{\mu-s} |\log h|^{\frac{1}{2}} \|v/\delta^s\|_{W^{\mu,\infty}(\Omega)}, \quad (4.25)$$

with $C_2 = C_2(\Omega, d, s, \mu) > 0$.

Proof. Let us first note that we can write

$$v - J_h v = \delta^s E_\alpha r_\Omega E_\mu \frac{v}{\delta^s} - \delta^s E_\alpha r_\Omega I_h E_\mu \frac{v}{\delta^s} = \delta^s E_\alpha r_\Omega \left(E_\mu \frac{v}{\delta^s} - I_h E_\mu \frac{v}{\delta^s} \right).$$

Therefore, for all $\alpha \in (s, \min\{\mu, 1\}]$, we can use Lemma B.2 to get

$$\begin{aligned} |v - J_h v|_{H^s(\mathbb{R}^d)} &\leq \|\delta^s\|_{L^\infty(\mathbb{R}^d)} \left| E_\alpha r_\Omega \left(E_\mu \frac{v}{\delta^s} - I_h E_\mu \frac{v}{\delta^s} \right) \right|_{H^s(\mathbb{R}^d)} \\ &\quad + |\delta^s|_{H^s(\mathbb{R}^d)} \left\| E_\alpha r_\Omega \left(E_\mu \frac{v}{\delta^s} - I_h E_\mu \frac{v}{\delta^s} \right) \right\|_{L^\infty(\mathbb{R}^d)} \\ &\lesssim \frac{\|\delta^s\|_{L^\infty(\mathbb{R}^d)}}{\sqrt{\alpha - s}} \left\| E_\alpha r_\Omega \left(E_\mu \frac{v}{\delta^s} - I_h E_\mu \frac{v}{\delta^s} \right) \right\|_{W^{\alpha,\infty}(\mathbb{R}^d)} \\ &\quad + |\delta^s|_{H^s(\mathbb{R}^d)} \left\| E_\mu \frac{v}{\delta^s} - I_h E_\mu \frac{v}{\delta^s} \right\|_{W^{\alpha,\infty}(\Omega)} \\ &\lesssim \frac{\|\delta^s\|_{L^\infty(\mathbb{R}^d)}}{\sqrt{\alpha - s}} \left\| E_\mu \frac{v}{\delta^s} - I_h E_\mu \frac{v}{\delta^s} \right\|_{W^{\alpha,\infty}(\Omega)} \\ &\quad + |\delta^s|_{H^s(\mathbb{R}^d)} \left\| E_\mu \frac{v}{\delta^s} - I_h E_\mu \frac{v}{\delta^s} \right\|_{W^{\alpha,\infty}(\Omega)} \\ &\leq \frac{\|\delta^s\|_{L^\infty(\mathbb{R}^d)} + |\delta^s|_{H^s(\mathbb{R}^d)}}{\sqrt{\alpha - s}} \left\| E_\mu \frac{v}{\delta^s} - I_h E_\mu \frac{v}{\delta^s} \right\|_{W^{\alpha,\infty}(\Omega)}, \end{aligned}$$

where we have used the symbol $\lesssim$ to express that the inequality holds up to a positive constant that depends only on Ω, d, s and μ . Due to Lemma 4.6 we have that

$$\left\| E_\mu \frac{v}{\delta^s} - I_h E_\mu \frac{v}{\delta^s} \right\|_{W^{\alpha,\infty}(\Omega)} \lesssim h^{\mu-\alpha} \left\| E_\mu \frac{v}{\delta^s} \right\|_{W^{\mu,\infty}(\mathbb{R}^d)} \lesssim h^{\mu-\alpha} \left\| \frac{v}{\delta^s} \right\|_{W^{\mu,\infty}(\Omega)}.$$

The proof of (4.24) is completed. For (4.25), it is enough to take the sequence $\alpha_h = s + \frac{1}{2|\log h|}$ for h small enough such that $\alpha_h \in (s, \min\{\mu, 1\}]$, and use (4.24). $\square$

We are now ready to present the main convergence results. First, in Theorem 4.8 we prove a general error estimate in $H^s(\mathbb{R}^d)$ seminorm, depending on the regularity of u/δ^s and the boundary of the domain $\partial\Omega$. Subsequently, we apply the result, under suitable regularity of the domain and the right-hand side f , to obtain Corollary 4.9. Finally, in Theorem 4.11 we obtain an error estimate in the $L^2(\Omega)$ norm as well.

Theorem 4.8. Let $s \in (0, 1)$, $\partial\Omega \in C^{1,1}$, $\mu \in (s, 2]$, and δ satisfy (4.8) with $\sigma = \max\{1, \mu\}$. Let also u be the corresponding solution of (4.4), assume that $u/\delta^s \in W^{\mu,\infty}(\Omega)$, and V_h be given by (4.13) and let u_h be the solution of (4.14). Then, we have that

$$|u - u_h|_{H^s(\mathbb{R}^d)} \leq Ch^{\mu-s} |\log h|^{\frac{1}{2}} \|u/\delta^s\|_{W^{\mu,\infty}(\Omega)}, \quad (4.26)$$

where $C > 0$ is a constant independent of h . In particular, the maximal order $h^{2-s} |\log h|^{\frac{1}{2}}$ is achieved if $\mu = 2$, i.e., $u/\delta^s \in W^{2,\infty}(\Omega)$.

Proof. It is enough to combine (4.18) with the competitor estimate of (4.19) and (4.25) to get

$$|u - u_h|_{H^s(\mathbb{R}^d)} = \inf_{v_h \in V_h} |u - v_h|_{H^s(\mathbb{R}^d)} \leq |u - J_h u|_{H^s(\mathbb{R}^d)},$$

and hence we arrive at the desired error estimate (4.26). $\square$

Corollary 4.9. Let $s \in (0, 1)$, $\gamma \in (s, 3)$ such that $\gamma, \gamma \pm s \notin \mathbb{N}$, $f \in W^{\gamma-s,\infty}(\Omega)$, $\partial\Omega \in C^{\gamma+1} \cap C^{1,1}$, and suppose that (4.8) holds with $\sigma = \gamma + 1$. Let u be the corresponding solution of (4.4), V_h be given by (4.13), and u_h be the solution of (4.14). Then, we have that

$$|u - u_h|_{H^s(\mathbb{R}^d)} \leq Ch^{\min\{2-s, \gamma-s\}} |\log h|^{\frac{1}{2}} \|f\|_{W^{\gamma-s,\infty}(\Omega)}, \quad (4.27)$$

where C does not depend on h .

Proof. Let us first notice that by [152, Proposition 1.1] we have $u \in C^s(\mathbb{R}^d)$ and

$$\|u\|_{W^{s,\infty}(\mathbb{R}^d)} \leq C_{\Omega,s} \|f\|_{L^\infty(\Omega)}, \quad (4.28)$$

where $C_{\Omega,s}$ is a positive constant depending only on the domain Ω and s . Applying the results of [1], summarised in (4.12), we have $u/\delta^s \in W^{\gamma,\infty}(\Omega)$ with the inequality

$$\|u/\delta^s\|_{W^{\gamma,\infty}(\Omega)} \leq C_{\Omega,d,s,\gamma} (\|f\|_{W^{\gamma-s,\infty}(\Omega)} + \|u\|_{L^\infty(\mathbb{R}^d)}),$$

for a positive constant $C_{\Omega,d,s,\gamma}$ depending only on Ω, d, s and γ . Inequality (4.28) therefore implies

$$\|u/\delta^s\|_{W^{\gamma,\infty}(\Omega)} \leq C_{\Omega,d,s,\gamma} \|f\|_{W^{\gamma-s,\infty}(\Omega)}. \quad (4.29)$$

We can therefore apply Theorem 4.8 with $\mu = \min\{\gamma, 2\}$, combining (4.26) with (4.29) to get the final result (4.27). $\square$

The standard approach to translate this H^s -rate to an improved L^2 -rate is to use an Aubin–Nitsche duality argument. The idea is to consider $e_h = u - u_h$ and note that for any $w_h \in V_h$ we have that

$$a_s(e_h, w_h) = a_s(u, w_h) - a_s(u_h, w_h) = \int_{\Omega} f(x) w_h(x) dx - \int_{\Omega} f(x) w_h(x) dx = 0.$$

Thus, given any ϕ_h , we consider the problem

$$(-\Delta)^s \psi_h = \phi_h \text{ in } \Omega, \quad \psi_h = 0 \text{ in } \mathbb{R}^d \setminus \Omega, \quad (4.30)$$

and note that for any $w_h \in V_h$, using the weak formulation of (4.30), we have that

$$\int_{\Omega} e_h(x) \phi_h(x) \, dx = a_s(e_h, \psi_h) = a_s(e_h, \psi_h - w_h) \leq |e_h|_{H^s(\mathbb{R}^d)} |\psi_h - w_h|_{H^s(\mathbb{R}^d)}.$$

Therefore, we get the following result

$$\int_{\Omega} e_h(x) \phi_h(x) \, dx \leq |e_h|_{H^s(\mathbb{R}^d)} \inf_{w_h \in V_h} |\psi_h - w_h|_{H^s(\mathbb{R}^d)}. \quad (4.31)$$

Due to C  a's lemma, Lemma 4.4, the infimum on the right-hand side is attained at the numerical solution of (4.30).

Remark 4.10. An interesting open question is whether Corollary 4.9 could be improved for $f \in L^2(\Omega)$ to a result analogous to the classical case $s = 1$, i.e.,

$$|u - u_h|_{H^s(\mathbb{R}^d)} \leq Ch^s |\log h|^\kappa \|f\|_{L^2(\Omega)}.$$

In the spirit of Theorem 4.8, this would mean that u/δ^s has “ $2s$ derivatives”. If this were the case we could prove, using $\phi_h = e_h$ and (4.31), an improved L^2 -error estimate of order h^2 , which is consistent with the rates suggested by the numerical experiments that we report in the following section.

Theorem 4.11. *Let the hypotheses of Corollary 4.9 hold. Additionally assume that $\partial\Omega \in C^{2,1}$. Then we have that*

$$\|u - u_h\|_{L^2(\mathbb{R}^d)} \leq Ch^{\min\{2-s, \gamma-s\} + \alpha} |\log h|^{\frac{3}{4}} \|f\|_{W^{\gamma-s, \infty}(\Omega)} \quad \text{for all } \alpha \in \left(0, s \frac{4-2s}{4+d}\right),$$

where $C > 0$ is a constant that does not depend on h .

Proof. Let $e_h = u - u_h$. Using the Fourier transform $\mathcal{F}$, let us consider

$$\phi_h := \mathcal{F}^{-1}[(1 + |\xi|^2)^{-t} \mathcal{F}[e_h]].$$

This corresponds to applying the operator $(I - \Delta)^{-t}$ in $\mathbb{R}^d$ to e_h . Let us also consider the following equivalent norm in $H^r(\mathbb{R}^d)$ for any $r \in \mathbb{R}$, given by

$$\|v\|_{H^r(\mathbb{R}^d)} := \|(1 + |\xi|^2)^{r/2} \mathcal{F}[v]\|_{L^2(\mathbb{R}^d)};$$

for a discussion on the equivalence between this norm and $|\cdot|_{H^r(\mathbb{R}^d)}$ we refer to [88, Proposition 3.3 and 3.4]. We deduce, by Plancherel's theorem, that $\phi_h \in H^{s+2t}(\mathbb{R}^d)$ and $\|\phi_h\|_{H^{s+2t}(\mathbb{R}^d)} = \|e_h\|_{H^s(\mathbb{R}^d)}$. Thus, by Morrey's inequality, we have that $\phi_h \in W^{s+2t-\frac{d}{2}, \infty}(\Omega)$ provided that $s + 2t - \frac{d}{2} > 0$. In particular

$$\|\phi_h\|_{W^{s+2t-\frac{d}{2}, \infty}(\Omega)} \leq C \|\phi_h\|_{H^{s+2t}(\mathbb{R}^d)} = C \|e_h\|_{H^s(\mathbb{R}^d)}, \quad \text{for all } t > \frac{d-2s}{4},$$

with C a generic positive constant. Let us now consider the WFEM solution corresponding to (4.30), that is the solution to the problem

$$\text{Find } \Psi_h \in V_h \text{ such that } a_s(\Psi_h, v_h) = \int_{\Omega} \phi_h(x) v_h(x) dx \text{ for all } v_h \in V_h.$$

We use now Corollary 4.9 with $\bar{\gamma} = 2s + 2t - \frac{d}{2}$, provided t is such that $\bar{\gamma}, \bar{\gamma} \pm s \notin \mathbb{N}$, and $0 < \bar{\gamma} - s < 2 - s$ to get

$$|\psi_h - \Psi_h|_{H^s(\mathbb{R}^d)} \leq Ch^{\bar{\gamma}-s} |\log h|^{\frac{1}{2}} \|\phi_h\|_{W^{\bar{\gamma}-s, \infty}} \leq Ch^{\bar{\gamma}-s} |\log h|^{\frac{1}{2}} |e_h|_{H^s(\mathbb{R}^d)}$$

where we have used that $\bar{\gamma} - s = s + 2t - \frac{d}{2}$. Note that we have used here the hypothesis $\partial\Omega \in C^{2,1}$. On the other hand, we can use Parseval's identity and proceed as in (4.31) to conclude that

$$\begin{aligned} \|e_h\|_{H^{-t}(\mathbb{R}^d)}^2 &= \int_{\mathbb{R}^d} e_h(x) \phi_h(x) dx = \int_{\Omega} e_h(x) \phi_h(x) dx = a_s(e_h, \psi_h) = a_s(e_h, \psi_h - \Psi_h) \\ &\leq |e_h|_{H^s(\mathbb{R}^d)} |\psi_h - \Psi_h|_{H^s(\mathbb{R}^d)} \\ &\leq Ch^{\bar{\gamma}-s} |\log h|^{\frac{1}{2}} |e_h|_{H^s(\mathbb{R}^d)}^2. \end{aligned}$$

Finally, let us note that with our chosen norms we have the following interpolation inequality if $-t\theta + s(1-\theta) = 0$ (i.e. $\theta = \frac{s}{s+t}$):

$$\begin{aligned} \|e_h\|_{L^2(\mathbb{R}^d)} &\leq \|e_h\|_{H^{-t}(\mathbb{R}^d)}^{\theta} \|e_h\|_{H^s(\mathbb{R}^d)}^{1-\theta} \\ &\leq Ch^{\frac{\theta}{2}(\bar{\gamma}-s)} |\log h|^{\frac{\theta}{4}} |e_h|_{H^s(\mathbb{R}^d)}. \end{aligned}$$

Summarizing, we have obtained that

$$\|e_h\|_{L^2(\mathbb{R}^d)} \leq Ch^{\frac{1}{2} \frac{s}{s+t} (\bar{\gamma}-s)} |\log h|^{\frac{1}{4} \frac{s}{s+t}} |e_h|_{H^s(\mathbb{R}^d)}$$

with $\bar{\gamma} = 2s + 2t - \frac{d}{2}$ provided t is such that $\bar{\gamma}, \bar{\gamma} \pm s \notin \mathbb{N}$, and $0 < \bar{\gamma} - s < 2 - s$. Note that, in particular, we have

$$\|e_h\|_{L^2(\mathbb{R}^d)} \leq Ch^{\frac{1}{2} \frac{s}{s+t} (s+2t-\frac{d}{2})} |\log h|^{\frac{1}{4} \frac{s}{s+t}} |e_h|_{H^s(\mathbb{R}^d)}$$

for almost every $t \in (\frac{d-2s}{4}, \frac{d-4s+4}{4})$. This implies

$$\|e_h\|_{L^2(\mathbb{R}^d)} \leq Ch^{\alpha} |\log h|^{\frac{1}{4}} |e_h|_{H^s(\mathbb{R}^d)}$$

for almost every $\alpha \in (0, s \frac{4-2s}{4+d})$. For the remaining $\alpha \in (0, s \frac{4-2s}{4+d})$ we can pick $\alpha_1, \alpha_2 \in (0, s \frac{4-2s}{4+d})$ with $\alpha_1 < \alpha < \alpha_2$ where the result holds, write $\alpha = (1-\theta)\alpha_1 + \theta\alpha_2$ with $\theta \in (0, 1)$ and then use the fact that

$$\begin{aligned} \|e_h\|_{L^2(\mathbb{R}^d)} &= \|e_h\|_{L^2(\mathbb{R}^d)}^{1-\theta} \|e_h\|_{L^2(\mathbb{R}^d)}^{\theta} \\ &\leq \left(C(\alpha_1) h^{\alpha_1} |\log h|^{\frac{1}{4}} |e_h|_{H^s(\mathbb{R}^d)} \right)^{1-\theta} \left(C(\alpha_2) h^{\alpha_2} |\log h|^{\frac{1}{4}} |e_h|_{H^s(\mathbb{R}^d)} \right)^{\theta} \\ &= C(\alpha_1)^{1-\theta} C(\alpha_2)^{\theta} h^{\alpha} |\log h|^{\frac{1}{4}} |e_h|_{H^s(\mathbb{R}^d)}. \end{aligned}$$

Applying the estimate in Corollary 4.9 we get the result. $\square$

Table 4.1: Convergence rates corresponding to Figure 4.4(a)

s	0.1	0.2	0.4	0.6
observed $h = 2^{-2}$	1.9914	1.87737	1.65643	1.42484
observed $h = 2^{-3}$	1.86733	1.73141	1.62081	1.430124
observed $h = 2^{-4}$	1.83477	1.73966	1.52709	1.38995
predicted	1.9	1.8	1.6	1.4

4.4 Numerical experiments

We now present numerical experiments for our method in one dimension. We omit here a discussion on how one computes in practice the stiffness matrix A_s in (4.16); this is a non-trivial matter as its entries $(A_s)_{i,j}$ involve the bilinear form $a_s(\cdot, \cdot)$ (5) and therefore a detailed treatment of this topic is deferred to the following and last chapter. For the purposes of the current chapter, we focus only on the spatial convergence in h of a WFEM approximation.

Let u^* be the explicit solution in (4.5) with $d = 1$, $R = 1$, and $x_0 = 0$, i.e., $\Omega = (-1, 1)$ and $f = 1$. In this case we can take $\Omega_h = \Omega$. In Figure 4.3, we can first qualitatively observe the improvement in the interpolation between $I_h u^*$ (piece-wise linear interpolation) and $J_h u^*$ (our tailored interpolation) for different choices of the regularised version of d_Ω , denoted by δ throughout the chapter, and a fixed h .

Although the overall solutions in Figures 4.3(a) to (c), appear similar a closer inspection near the boundary (see Figures 4.3(d) to (f)) clearly reveals the remarkable capability of WFEM in capturing the behaviour of the exact solution. In particular, we observe that the solution obtained with WFEM closely matches the profile of u^* near the boundary. Since the $J_h u^*$ associated to $\delta(x) = 1 - |x|^2$ and $\delta(x) = 1 - |x|^4$ seem equivalent in Figures 4.3(d) to (f), we provide Figures 4.3(g) to (i) where we show $I_h(u^*/\delta^s) = J_h(u^*)/\delta^s$.

In Figure 4.4 we validate the theoretical results that we have presented in Theorem 4.8, Corollary 4.9 and Theorem 4.11. In particular, with the choice of $f = 1$ we put ourselves in the case of maximal H^s -rate of Corollary 4.9, i.e., $h^{2-s}|\log h|^{\frac{1}{2}}$. As shown in Figure 4.4(a) the observed convergence rates match the theoretical prediction, with the observed slope of every convergence line in log scale for different s being approximately $2 - s$. Figure 4.4(b) instead is linked to the fact that, even though we are only able to prove Theorem 4.11, we would expect the convergence to be quadratic in $L^2(\Omega)$ norm.

In Table 4.1 we report the observed convergence rates for the example corresponding to the slope of the segments in Figure 4.4(a). The values have been computed using the incremental ratio formula $(\log |e_h|_{H^s(\mathbb{R}^d)} - \log |e_{2h}|_{H^s(\mathbb{R}^d)})/(\log h - \log 2h)$, where we recall that $e_h = u_h - u^*$.

Let us now consider the solution of (4.1) on $\Omega = (-1, 1)$, for f given by (4.6), that is $u(x) = (1 - |x|^2)_+$, which clearly does not behave like d_Ω^s . Since $u \not\geq c\delta^s$, it follows from (4.11)

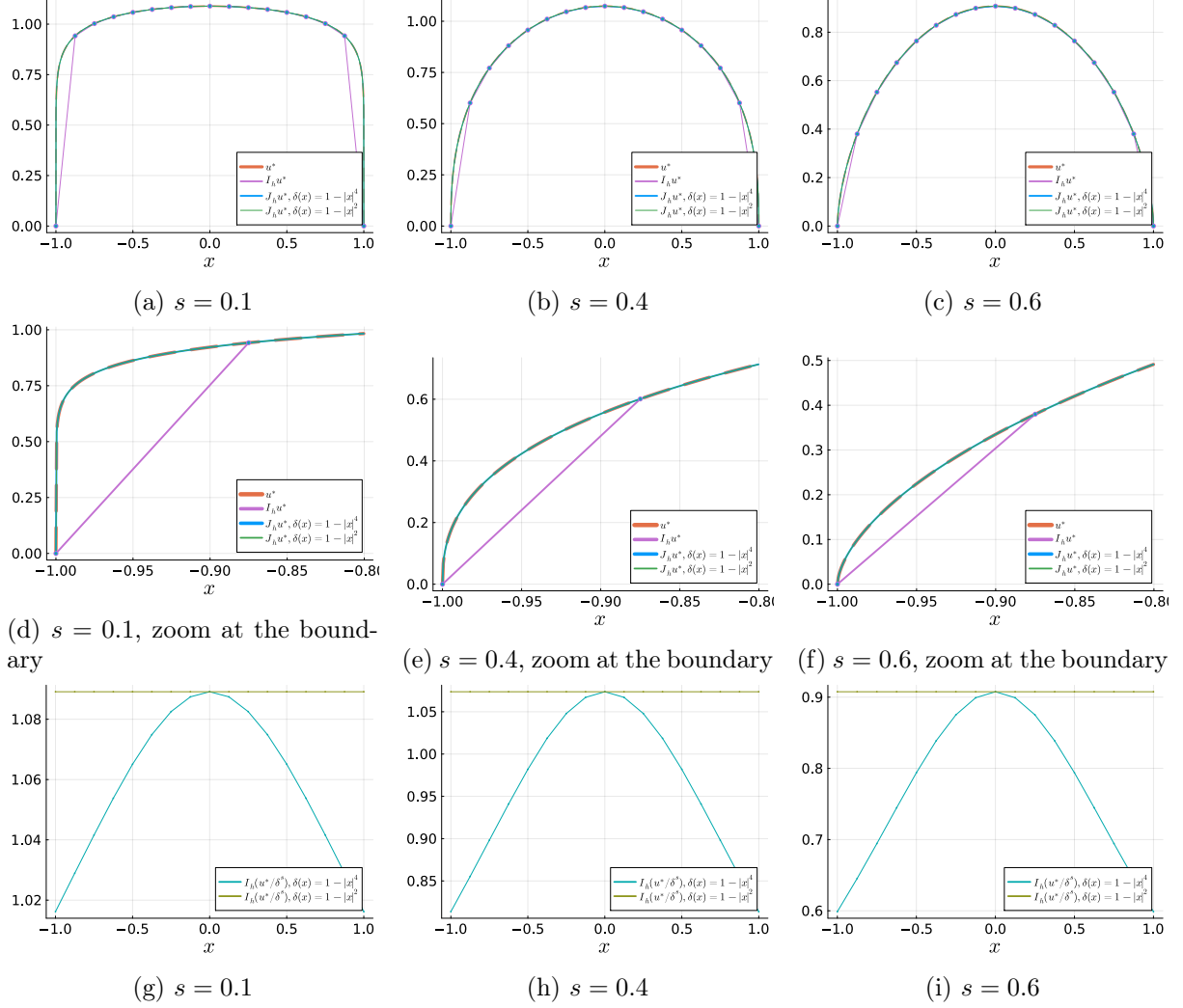
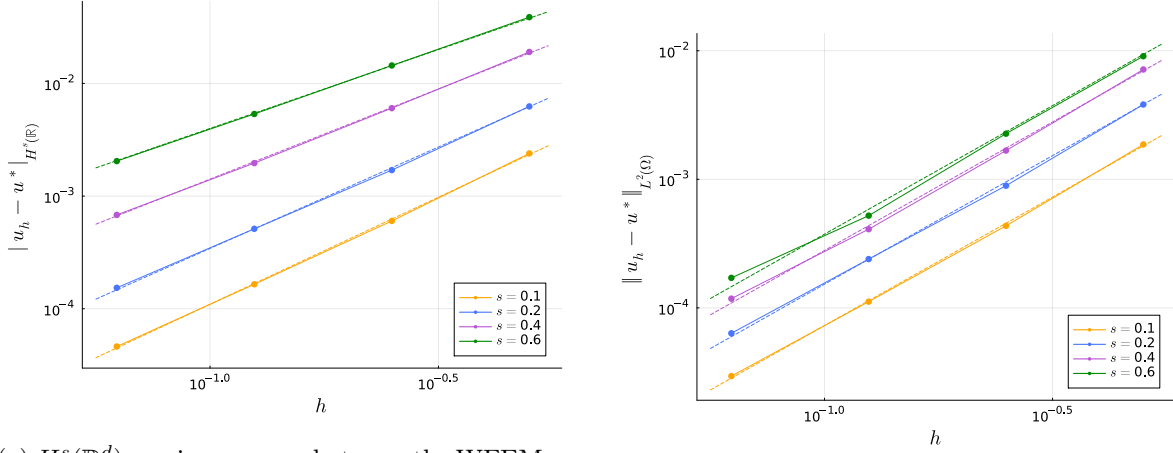


Figure 4.3: Fractional Dirichlet problem (4.1); comparison between explicit solution (4.5), piecewise linear interpolation $I_h u^*$ and $J_h u^*$, defined in (4.19), for different choices of the function δ . $\Omega = \Omega_h = (-1, 1)$, uniform meshes with $h = |\Omega|/2^4$.



(a) $H^s(\mathbb{R}^d)$ -seminorm error between the WFEM approximation and the solution. Dashed lines: $g(h) = Ch^{2-s}$.

(b) $L^2(\Omega)$ error between the WFEM approximation and the solution. Dashed lines: $g(h) = Ch^2$.

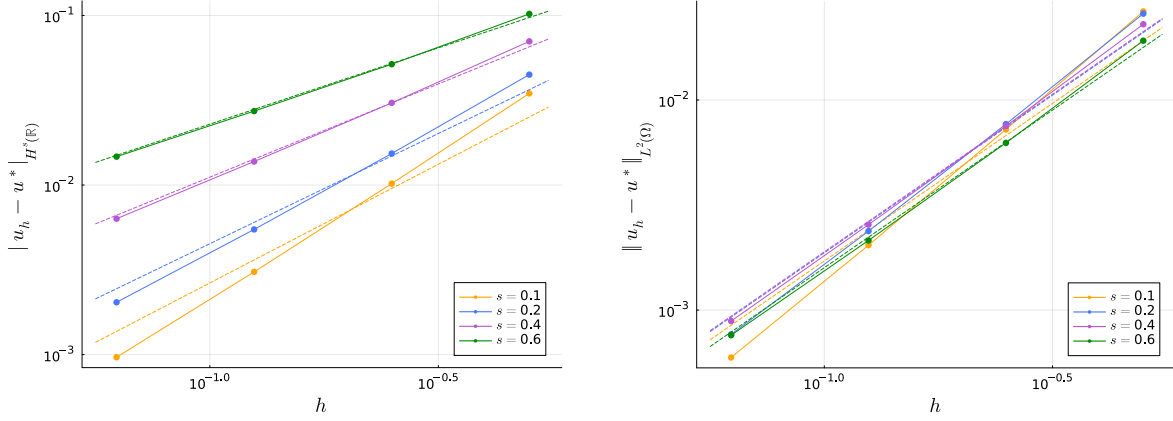
Figure 4.4: Fractional Dirichlet problem (4.1); WFEM computational errors. The computational domain is $\Omega = \Omega_h = (-1, 1)$, $f = 1$ and u^* is given by (4.5). The numerical tests were performed with meshes of equally spaced nodes, with mesh size $h = 2^{-m}$ for $m = 1, \dots, 4$. As regularised distance, satisfying (4.8), $\delta(x) = 1 - |x|^4$ was used.

that f must change sign. Moreover, as we have already mentioned, for $s \geq 1/2$ and $d = 1$, one has $f \notin L^\infty(\Omega)$. This type of right-hand side has been used for validation of FEM schemes with piece-wise linear functions in [42], where the authors report a rate of $h^{\frac{3}{2}-s}$. Since $u \in C^\infty(\bar{\Omega})$ it is natural that piecewise linear basis functions yield good approximation.

Since $u/\delta^s \sim \delta^{1-s}$, Theorem 4.8 yields at most a rate of h^{1-2s} when $s \in (0, 1/2)$ (the same range where $f \in L^\infty(\Omega)$). This limitation is related to the fact that optimal rates for smooth f rely on $C^{s+\varepsilon}$ -regularity to control H^s -errors.

Although this goes against the philosophy of our choice of basis, we have performed numerical experiments with this right-hand side for completeness. In order to approximate the right-hand side of (4.14) we performed the experiments in $\Omega = \Omega_h = (-1 + \varepsilon, 1 - \varepsilon)$, $\varepsilon = 10^{-10}$. Quite surprisingly, the observed rates in Figure 4.5 match those in [42] for $s \in [1/2, 1)$ and even improve them for $s \in (0, 1/2)$. An interesting open question is to rigorously prove this behaviour.

In Table 4.2 we report the observed convergence rates for the example corresponding to the slope of the segments in Figure 4.5(a). The values have been computed using the incremental ratio formula $(\log e_h - \log e_{2h})/(\log h - \log 2h)$.



(a) $H^s(\mathbb{R}^d)$ -seminorm error between the WFEM approximation and the solution. The dashed lines correspond to $Ch^{\frac{3}{2}-s}$.

(b) $L^2(\Omega)$ error between the WFEM approximation and the solution. The dashed lines correspond to $Ch^{\frac{3}{2}}$.

Figure 4.5: Fractional Dirichlet problem (4.1); WFEM computational errors. The computational domain is $\Omega = (-1 + \varepsilon, 1 - \varepsilon)$, with $\varepsilon = 10^{-10}$, f is given by (4.6) and $u^* = (1 - |x|^2)_+$. The numerical tests were performed with meshes of equally spaced nodes, with mesh size $h = (1 - \varepsilon)2^{-m}$ for $m = 1, \dots, 4$. As regularised distance, satisfying (4.8), $\delta(x) = 1 - |x|^4$ was used.

Table 4.2: Convergence rates corresponding to Figure 4.5 (a)

s	0.1	0.2	0.4	0.6
observed $h = (1 - \varepsilon)2^{-2}$	1.7669	1.54577	1.20472	0.985209
observed $h = (1 - \varepsilon)2^{-3}$	1.72902	1.48647	1.14931	0.919176
observed $h = (1 - \varepsilon)2^{-4}$	1.67254	1.42748	1.11971	0.892579
predicted in [42]	1.4	1.3	1.1	0.9

Yes, we shall live, Uncle Vanya.

Anton Čechov (1860– 1904), “Uncle Vanya”

5

Variational crimes in the finite element method for the integral fractional Laplacian

In the final chapter of the thesis we disclose and discuss an issue related to solving the fractional Dirichlet problem (4.1), that is of particular importance when using a WFEM approach. As we mentioned in Section 4.4 of Chapter 4, we deliberately postponed its analysis in order to keep the previous chapter concise and focused on the spatial error of WFEM. The matter that we are going to treat now, constitutes a challenge that is more generally related to any approximation of the integral fractional Laplacian. As in many differential problems, the computation of the bilinear form arising from a weak formulation is a crucial aspect for a numerical approximation. In fact, in our case the bilinear form $a_s(\cdot, \cdot)$ defined in (5) is used in both the weak formulation of the fractional Dirichlet problem (4.4) and in its finite element discretization (4.14); more specifically, in the linear system (4.16) the computation of the stiffness matrix A_s clearly involves $a_s(\cdot, \cdot)$. The presence of the integral fractional Laplacian however introduces an additional layer of complexity: the nature of the bilinear form (5) involving a double integral over $\mathbb{R}^d$ does not allow to compute exactly $(A_s)_{i,j}$, even for standard and simple basis functions.

This difficulty in the computation of bilinear forms has long been recognised in numerical analysis, even for local differential problems (for example $(v, w) \mapsto (M \nabla v, \nabla w)$ with M not constant). The foundational paper by G. Strang [168] studied the issue of not computing a bilinear form exactly, by committing a so-called “variational crime”, that is, replacing the bilinear form by a suitable approximation of it.

The computation of the stiffness matrix for a piecewise linear finite element approximation of the fractional Dirichlet problem is an issue that has been explored in some of the previous works that we cited. In [5, Section 5] the authors discussed their strategy for computing the

stiffness matrix, that was later explicitly presented in a MATLAB implementation in [4] (see also [160, Chapter 5]), however without going into the details of the variational crime that one commits in approximating the entries of the matrix and of the interaction between the finite element discretization and the approximation of the bilinear form, as well as the additional computational cost that this implies. Later, the authors of [42] proposed an approximation of the integral fractional Laplacian using an explicit integral representation formula that allows one to rewrite the bilinear form a_s in the form $a_s(\phi, \psi) = c_s \int_0^\infty t^{2-2s} ((-\Delta)(I - t^2 \Delta)^{-1} \phi, \psi) \frac{dt}{t}$; in their article they fully discuss the variational crimes committed in approximating such a formula, including a Strang-type lemma, under the assumption that the approximated bilinear form is coercive; the recent work [13] also adopted a similar strategy for a different approximation based on hp -FEM.

As a matter of fact, even in our case, we had to introduce a computable approximation of the bilinear form a_s ; this was needed for example for the computation of the results reported in Section 4.4 of the previous chapter. Let us then denote by $a_{s,\rho}$ the approximation of a_s , for a parameter $\rho \geq 0$. Hence, the approximated discrete problem becomes

$$\text{Find } u_{h,\rho} \in V_h \text{ such that } a_{s,\rho}(u_{h,\rho}, v_h) = \int_\Omega f v_h \, dx \quad \text{for all } v_h \in V_h. \quad (5.1)$$

Consequently, in the linear system that one actually solves, the stiffness matrix would have entries $(A_s^\rho)_{i,j} = a_{s,\rho}(\phi_j, \phi_i)$. While the error in h is controlled by estimates in the spirit of Cea's lemma, as the ones that we proved in Chapter 4 (Lemma 4.4 and Theorem 4.8), our aim in this chapter is to study the error in ρ and how it affects the overall approximation of u through $u_{h,\rho}$. Citing Strang [168], “*We want [...] to find out which violations of the rules still yield a convergent approximation. In other words we want to find out whether or not crime pays; fortunately for the finite element method, it often does.*”

We will first provide a general Strang-type lemma to illustrate the effect of approximating a_s and then describe the implementation of an explicit approximation $a_{s,\rho}$ that complements our work for the method described in Chapter 4 and fully explains how we computed the results reported there. For the purposes of our work, we will be particularly focused on the computational aspects of the approximation $a_{s,\rho}$ and how one can develop an efficient implementation strategy for it. Indeed, the approximation of the bilinear form is not only a delicate point in terms of the overall numerical approximation, but also in terms of the total computational cost that is required. As noted previously, the original bilinear form a priori involves a double integral on the whole of $\mathbb{R}^d \times \mathbb{R}^d$ and a singularity due to the presence of the term $|x - y|^{-d-2s}$; both of these facts are factors that strongly influence a performant computation of $a_{s,\rho}(\cdot, \cdot)$.

The full numerical discretizations of $a_s(\cdot, \cdot)$ available in the literature, mainly [5, 42, 13] are fairly elaborate to implement. For the purposes of our work, we aim to discuss the most naïve

of the possible approximations, given by a piecewise constant interpolation. Let $0 < \rho \ll 1$, $x_k = \rho k$ for $k \in \mathbb{Z}^d$ and $\varepsilon_\rho \in [\rho, 1)$, $R_\rho \in (1, \infty]$, we consider

$$a_{s,\rho}(\phi, \psi) := \frac{C_{d,s}}{2} \sum_{\substack{x_k, x_\ell \in Q_{R_\rho} \\ |x_k - x_\ell|_\infty \geq \varepsilon_\rho}} \frac{(\phi(x_k) - \phi(x_\ell))(\psi(x_k) - \psi(x_\ell))}{|x_k - x_\ell|^{d+2s}} \rho^{2d}, \quad (5.2)$$

where we denote the cube $Q_R := [-R, R]^d$. In fact, we admit the use of $R_\rho = \infty$, for which (5.2) is computable as we will discuss later in the chapter. Loosely speaking, the quadrature is constructed through a piecewise constant approximation on d -dimensional cubes centred at the points x_k and, since we are working on cubes, we use the ℓ_∞ -distance

$$|x|_\infty = \max_{i=1, \dots, d} |x_i| \text{ for } x \in \mathbb{R}^d;$$

recall that this is equivalent to the ℓ_2 distance.

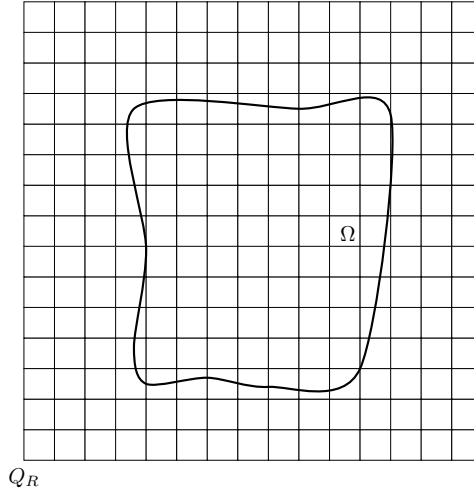


Figure 5.1: Quadrature $Q_R = [-R, R]^d \supset \Omega$

In spite of its simplicity, the approximation (5.2) presents interesting computational challenges; in the following we will discuss how one can use FFT and the Riemann or Epstein zeta function to make its implementation efficient.

Remark 5.1. Before proceeding further, we comment on the computation of the terms $\int_\Omega f \zeta_i \, dx$, where ζ_i , $i = 1, \dots, N_h$, are the basis functions of the finite dimensional space V_h ; these terms are the entries F_i , $i = 1, \dots, N_h$, of the right-hand side vector F in the finite element approximation of the fractional Dirichlet problem in the linear system form (4.16).

In a standard finite element setting the elements of a basis for V_h are (for example) continuous piecewise linear functions and they are typically chosen as a nodal basis; with this choice the right-hand side vector F in (4.16) is assembled straightforwardly (see [5, Section 5]). In the case of WFEM, the approximation of the entries $\int_\Omega f \zeta_i \, dx$ is a nontrivial matter and in general

it requires committing another variational crime, approximating them with a proper quadrature rule. However, since this variational crime concerns purely numerical integration of a L^∞ function defined on a bounded domain and it does not relate to the fractional Laplacian, we will omit its discussion in order to keep the chapter focused on the variational crime committed in the integrals that directly involve the definition of the integral fractional Laplacian. A simple strategy to circumvent the issue is to employ a piecewise constant approximation for these terms, based on a grid that is fine enough to suppress the associated quadrature error. For WFEM the elements of $\{\zeta_i\}_{i=1}^{N_h}$ have only C^s regularity because $\zeta_i \in \delta^s \text{PL}(\mathcal{T}_h)$, where δ^s is the regularised distance function defined in (4.8). Numerical integration of Hölder continuous functions with standard techniques usually requires a fine grid as the low regularity of the integrand slows down convergence: in fact, using quadrature rules based on function values at n points, the integral of a C^s function is usually approximated with error of order $\mathcal{O}(n^{-s/d})$ (see [79, Section 2.1] or more recently [15]).

We now present a Strang-type lemma. We recall that for $a_s(\cdot, \cdot)$ we have continuity and coercivity, namely

$$\alpha_* \|v\|_V^2 \leq a_s(v, v) \quad \text{and} \quad a_s(v, w) \leq M \|v\|_V \|w\|_V \quad \text{for all } v, w \in V, \quad (5.3)$$

for positive constants α_* and M and $V = H^s(\mathbb{R}^d)$ defined in (4.2)

To avoid hiding the dependence of the coercivity constant on the regularity of the basis functions and the triangulation, we state a version of Strang's first lemma where we keep track of all the dependences following the classical proof.

Let V_h be a finite-dimensional subspace of $H_0^s(\Omega)$. First, let us state quantitatively the error between a_s and $a_{s,\rho}$ in the form

$$|a_s(\psi, \phi) - a_{s,\rho}(\psi, \phi)| \leq \omega_{a,X}(\rho) \|\psi\|_X \|\phi\|_X \quad (5.4)$$

where $\omega_{a,X}$ is a modulus of continuity, and X is a space of “higher regularity” functions such that $V_h \subset X \subset V$. Since V_h is finite-dimensional, let us consider the constant of norm-equivalence

$$\mathbf{E}(V_h, V, X) := \sup_{\substack{v_h \in V_h \\ v_h \neq 0}} \frac{\|v_h\|_X}{\|v_h\|_V}. \quad (5.5)$$

We will denote this constant by $\mathbf{E}_h$ for brevity. Following the classical proof, we have the following version of the classical Strang lemma.

Lemma 5.2 (Strang-type lemma). *Assume (5.3), and let u be the solution of (4.4), $u_{h,\rho}$ the solution of the approximate problem (5.1), and $\mathbf{E}_h = \mathbf{E}(V_h, V, X)$. Moreover, assume $\rho \in (0, \rho_1)$ so that $\frac{1}{\alpha_*} \mathbf{E}_h^2 \omega_{a,X}(\rho) < 1$. Then, the following a priori error estimate holds:*

$$\begin{aligned} & \left(1 - \frac{1}{\alpha_*} \mathbf{E}_h^2 \omega_{a,X}(\rho)\right) \|u - u_{h,\rho}\|_V \\ & \leq \inf_{v_h \in V_h} \left(\left(1 + \frac{M}{\alpha_*} + \frac{1}{\alpha_*} \omega_{a,X}(\rho) \mathbf{E}_h^2\right) \|u - v_h\|_V + \frac{1}{\alpha_*} \sup_{w_h \in V_h} \frac{|a_s(v_h, w_h) - a_{s,\rho}(v_h, w_h)|}{\|w_h\|_V} \right). \end{aligned} \quad (5.6)$$

Proof. Let $v_h \in V_h$ be fixed and let $w_{h,\rho} = u_{h,\rho} - v_h$. By the triangle inequality, we have that

$$\|u - u_{h,\rho}\|_V \leq \|u - v_h\|_V + \|v_h - u_{h,\rho}\|_V$$

and by coercivity of $a_s(\cdot, \cdot)$, (5.3),

$$\|w_{h,\rho}\|_V^2 \leq \frac{1}{\alpha_*} a_s(w_{h,\rho}, w_{h,\rho}) = \frac{1}{\alpha_*} a_{s,\rho}(w_{h,\rho}, w_{h,\rho}) + \frac{1}{\alpha_*} \tau(h, \rho),$$

where $\tau(h, \rho) = a_s(w_{h,\rho}, w_{h,\rho}) - a_{s,\rho}(w_{h,\rho}, w_{h,\rho})$ is the consistency term. Then we have

$$\begin{aligned} \|w_{h,\rho}\|_V^2 &\leq \frac{1}{\alpha_*} a_{s,\rho}(u_{h,\rho}, w_{h,\rho}) - \frac{1}{\alpha_*} a_{s,\rho}(v_h, w_{h,\rho}) + \frac{1}{\alpha_*} \omega_{a,X}(\rho) \|w_{h,\rho}\|_X^2 \\ &= \frac{1}{\alpha_*} \int_{\Omega} f w_{h,\rho} \, dx - \frac{1}{\alpha_*} a_{s,\rho}(v_h, w_{h,\rho}) + \frac{1}{\alpha_*} \omega_{a,X}(\rho) \mathbf{E}_h^2 \|w_{h,\rho}\|_V^2 \\ &= \frac{1}{\alpha_*} a_s(u, w_{h,\rho}) - \frac{1}{\alpha_*} a_{s,\rho}(v_h, w_{h,\rho}) + \frac{1}{\alpha_*} \omega_{a,X}(\rho) \mathbf{E}_h^2 \|w_{h,\rho}\|_V^2 \\ &= \frac{1}{\alpha_*} a_s(u - v_h, w_{h,\rho}) + \frac{1}{\alpha_*} a_s(v_h, w_{h,\rho}) - \frac{1}{\alpha_*} a_{s,\rho}(v_h, w_{h,\rho}) + \frac{1}{\alpha_*} \omega_{a,X}(\rho) \mathbf{E}_h^2 \|w_{h,\rho}\|_V^2. \end{aligned}$$

Hence, by continuity of $a_s(\cdot, \cdot)$, (5.3),

$$a_s(u - v_h, w_{h,\rho}) \leq M \|u - v_h\|_V \|w_{h,\rho}\|_V.$$

It also holds

$$\|w_{h,\rho}\|_V \leq \|u - v_h\|_V + \|u - u_{h,\rho}\|_V.$$

Combining the inequalities, dividing by $\|w_{h,\rho}\|_V$, and denoting $w_h = w_{h,\rho}$, we have

$$\begin{aligned} \|u_{h,\rho} - u\|_V &\leq \left(1 + \frac{M}{\alpha_*}\right) \|u - v_h\|_V + \frac{1}{\alpha_*} \frac{|a_s(v_h, w_h) - a_{s,\rho}(v_h, w_h)|}{\|w_h\|_V} \\ &\quad + \frac{1}{\alpha_*} \omega_{a,X}(\rho) \mathbf{E}_h^2 \|u - v_h\|_V + \frac{1}{\alpha_*} \omega_{a,X}(\rho) \mathbf{E}_h^2 \|u - u_{h,\rho}\|_V. \end{aligned}$$

Therefore, we have overall

$$\begin{aligned} \left(1 - \frac{1}{\alpha_*} \mathbf{E}_h^2 \omega_{a,X}(\rho)\right) \|u - u_{h,\rho}\|_V &\leq \left(1 + \frac{M}{\alpha_*} + \frac{1}{\alpha_*} \mathbf{E}_h^2 \omega_{a,X}(\rho)\right) \|u - v_h\|_V \\ &\quad + \frac{1}{\alpha_*} \frac{|a_s(v_h, w_h) - a_{s,\rho}(v_h, w_h)|}{\|w_h\|_V}. \end{aligned} \tag{5.7}$$

If in (5.7) we take the supremum over $w_h \in V_h$, followed by taking the infimum over $v_h \in V_h$, we get the result (5.6). $\square$

Corollary 5.3. *Under the hypotheses of Lemma 5.2, if we have an explicit modulus of continuity $\omega_u(h)$ such that*

$$\inf_{v_h \in V_h} \|u - v_h\|_V \leq \omega_u(h),$$

then

$$\left(1 - \frac{1}{\alpha_*} \mathbf{E}_h^2 \omega_{a,X}(\rho)\right) \|u - u_{h,\rho}\|_V \leq \left(1 + \frac{M}{\alpha_*} + \frac{2}{\alpha_*} \omega_{a,X}(\rho) \mathbf{E}_h^2\right) \omega_u(h) + \frac{1}{\alpha_*} \omega_{a,X}(\rho) \mathbf{E}_h^2 \|u\|_V. \quad (5.8)$$

If additionally we consider $\rho_h > 0$ be such that

$$\omega_{a,X}(\rho_h) \leq \alpha_* \frac{\min\{1, \omega_u(h)\}}{\mathbf{E}_h^2}, \quad (5.9)$$

and h be small enough so that $\omega_u(h) < 1$ then

$$\|u - u_{h,\rho_h}\|_V \leq \frac{1 + \frac{M}{\alpha_*} + \|u\|_V + 2\omega_u(h)}{1 - \omega_u(h)} \omega_u(h). \quad (5.10)$$

Proof. We have that

$$|a_s(v_h, w_h) - a_{s,\rho}(v_h, w_h)| \leq \omega_{a,X}(\rho) \mathbf{E}_h^2 \|v_h\|_V \|w_h\|_V$$

and using this in (5.6) we immediately get (5.8).

Finally, taking the correct scaling (5.9), a simple computation leads to (5.10). $\square$

From (5.6) we can see that the error is governed by a Strang type quantity measuring how well V_h approximates V and how well $a_{s,\rho}(\cdot, \cdot)$ approximates $a_s(\cdot, \cdot)$ on V_h . Moreover $\omega_{a,X}(\rho)$ plays a role of an amplification factor for the error. Notice that for a standard FEM the value of $\omega_u(h)$ is provided by (4.7), while for WFEM this is provided by Lemma 4.4, Theorem 4.8 and then Corollary 4.9.

In numerical experiments for WFEM, in order to observe the convergence rate in h , that is theoretically predicted by Theorem 4.8, one needs to use a sufficiently small value of ρ . In this way (5.10) can hold and the error $\|u - u_{h,\rho}\|_V$ will be controlled similarly to $\|u - u_h\|_V$ as if one could compute exactly the bilinear form $a_s(\cdot, \cdot)$; this is precisely the strategy that we used for all the results reported in the previous chapter.

Often the explicit dependence on the term $\mathbf{E}_h^2 \omega_{a,X}(\rho)$ is omitted in similar discussions of variational crimes; this is for example the case for the previously cited works [42, 13], where the authors assume that the approximation parameter for the bilinear form is chosen to be small enough to have coercivity of the approximated bilinear form and consequently apply what is referred to as first Strang lemma [74, Theorem 4.1.1]. We prefer to exploit the dependence on it because we believe this is of particular relevance to understand the effect of using a WFEM approach instead of a standard FEM: changing the function space for the basis functions of the finite element method clearly affects both $\mathbf{E}_h$ and $\omega_{a,X}(\rho)$, as they are defined in (5.4) and (5.5). Our aim is to study computationally the interplay between the approximation parameter ρ and the parameter h of the finite element discretization and we believe that in this way one can fully understand a further difficulty in using the weighted finite element method that we described in

the previous chapter: while for a standard piecewise linear approximation the error introduced by $a_{s,\rho}$ is often negligible, for WFEM the choice of the parameter ρ is always crucial to observe the superlinear convergence in h .

In fact, on a polytopal Lipschitz domain, using a piecewise linear approximation we have

$$V_h = \text{PL}(\mathcal{T}_h) \cap W_0^{1,\infty}(\Omega), \quad X = W_0^{1,\infty}(\Omega),$$

while in the setting that we described in Chapter 4 for WFEM a natural choice is

$$V_h = \delta^s \text{PL}(\mathcal{T}_h), \quad X = \delta^s W^{1,\infty}(\mathbb{R}^d).$$

These differences would clearly affect both E_h and $\omega_{a,X}(\rho)$ and, as we will see in the numerical experiments, we expect them to slow down the convergence in ρ for the case of WFEM with respect to a standard FEM approach. A close inspection of our formula for the quadrature (5.2) already gives some intuition about this fact and how it is specifically related to the singularity of the kernel in the expression for $a_s(\cdot, \cdot)$: having a piecewise Lipschitz basis allows the term at the numerator of (5.2) to better control the singularity at the denominator given by $|x_k - x_\ell|^{-d-2s}$ for x_k, x_ℓ points of the quadrature, whereas the use of a basis with generally only C^s regularity clearly makes this control weaker. From this observation, a lower convergence rate in ρ is expected when employing (5.2) for WFEM.

Remark 5.4. It is possible to show that, for our choice of the quadrature rule (5.2) (with $R_\rho \geq \rho^{-\frac{1-s}{s}}$ and $\varepsilon_\rho = \rho$), for $X = W^{1,\infty}(\Omega)$, for the term $\omega_{a,X}(\rho)$ in (5.4) one has

$$\omega_{a,W^{1,\infty}}(\rho) = \begin{cases} \rho & \text{if } s < \frac{1}{2}, \\ \rho |\log \rho| & \text{if } s = \frac{1}{2}, \\ \rho^{2(1-s)} & \text{if } s > \frac{1}{2}. \end{cases} \quad (5.11)$$

Extending and proving a similar estimate for $X = \delta^s W^{1,\infty}(\mathbb{R}^d)$ constitutes an open problem and a direction for future work. However, in the section containing numerical experiments, we will use the above estimate as a comparison for the observed convergence in ρ of our approximation (5.2) to validate our implementation.

5.1 Computational aspects

We now describe an efficient strategy to implement the approximated bilinear form $a_{s,\rho}(\cdot, \cdot)$ given by (5.2). Quite surprisingly, the implementation is simpler and more efficient when $R = \infty$. As we will show now, this apparently infinite sum can be computed in finitely many operations. Let us denote

$$K_\rho(|x|) = \frac{C_{d,s}}{2} \begin{cases} |x|^{-d-2s} & \text{if } |x|_\infty \geq \varepsilon_\rho \\ 0 & \text{otherwise.} \end{cases}$$

Expanding the sum in (5.2) for $R = \infty$, we have

$$\begin{aligned} a_{s,\rho}(\phi, \psi) &= \rho^{2d} \sum_{k,l \in \mathbb{Z}^d} (\phi(x_k) - \phi(x_l))(\psi(x_k) - \psi(x_l))K_\rho(|x_k - x_l|) \\ &= 2 \left(\rho^d \sum_{l \in \mathbb{Z}^d} K_\rho(|x_l|) \right) \left(\rho^d \sum_{k \in \mathbb{Z}^d} \phi(x_k)\psi(x_k) \right) \\ &\quad - 2\rho^d \sum_{k \in \mathbb{Z}^d} \phi(x_k) \left(\rho^d \sum_{l \in \mathbb{Z}^d} \psi(x_l)K_\rho(|x_k - x_l|) \right). \end{aligned}$$

When ϕ and ψ are supported inside Ω , all the sums above are finite except for

$$C_K := \rho^d \sum_{x_l \in \mathbb{Z}^d} K_\rho(|x_l|),$$

and this is the case for both FEM and WFEM. In dimension $d = 1$ we can take advantage of the Riemann zeta function

$$\zeta(s) = \sum_{k=1}^{\infty} \frac{1}{k^s}.$$

This function cannot be exactly evaluated, but there are sufficiently accurate numerical implementations available for scientific computing. For $d > 1$ the corresponding function is the so-called Epstein zeta function, which for our purposes can be simplified to

$$Z(d, \nu) = \sum_{k \in \mathbb{Z}^d \setminus \{0\}} |k|^{-\nu}, \quad \text{where } \nu > d;$$

notice that $Z(1, \nu) = 2\zeta(\nu)$. Numerical schemes for the computation of this constant have been recently developed. For both functions the available implementations are very efficient compared to the overall complexity of the algorithm for assembling the stiffness matrix $A_{s,\rho}$: the Riemann zeta function is computed in the order of ns, whereas the Epstein zeta function is evaluated in the order of μ s on a standard machine. Notice that, depending on the choice of ε_ρ , one only needs to remove a few summands from the zeta function

$$C_K = \frac{C_{d,s}}{2} \rho^{-2s} \left(Z(d, d+2s) - \sum_{\substack{k \in \mathbb{Z}^d \\ 0 < |k|_\infty < \frac{\varepsilon_\rho}{\rho}}} |k|^{-d-2s} \right); \quad (5.12)$$

in our experiments we will take $\varepsilon_\rho = \rho$, so there is no subtraction.

This observation comes with a great computational benefit: as a matter of fact, computing C_K using its definition for $R < \infty$ (for large values of R) is extremely costly as it would involve a loop over a large subset of $\mathbb{Z}^d$ to reach the required accuracy, while if we use the Riemann and Epstein zeta functions the computation of C_K ultimately comes down to a single evaluation of these functions, immensely reducing the total computational cost.

Lastly, we point out that the operation

$$\rho^d \sum_{l \in \mathbb{Z}^d} \psi(x_l) K_\rho(|x - x_l|) \quad (5.13)$$

is a convolution and can therefore be very efficiently computed using Fast Fourier Transform (FFT). This computation could be further speeded up by using GPUs, but we remark that in dimension $d = 1$ the convolution can be easily implemented through the use of symmetric Toeplitz matrices that allow a very efficient and convenient computation of FFT (see [112]).

Remark 5.5. Notice that in order to compute (5.13) for functions with $\text{supp}(\psi) \subset \Omega$ we only need values of K_ρ on the points $Y_\rho = \{y \in \rho\mathbb{Z}^d : |y| \leq \text{diam}(\Omega)\}$ and the evaluations of ψ at these points. These values can be pre-loaded into an array when creating the quadrature and used subsequently. In fact, for what we said before, it is worth storing the FFT of this array. This fact constitutes a great advantage in terms of storage: instead of allocating memory for the values at all the points inside a d dimensional cube $[-R, R]^d$ of size $R > 0$, we end up storing only those in Y_ρ .

5.2 Numerical experiments

The numerical experiments that we report below clarify the effect of committing a variational crime for the integral fractional Laplacian in (4.1); in our view, on the one hand they provide a deeper understanding of the convergence results depicted in Chapter 4 (for example in Figure 4.4) and at the same time they expose the price that one pays in reality for using a WFEM approach. Concurrently, in order to appreciate the potential advantage of using WFEM, we report also the convergence results that one would have in using a standard piecewise linear basis for the finite element method, employing the same quadrature rule (5.2). Our experiments are still done using the explicit solution u^* (4.5) and for WFEM we set $\delta(x) = 1 - |x|^4$ as regularised distance function.

At first, we validate our piecewise constant quadrature rule approximating $a_s(\cdot, \cdot)$. Since we have that $a_s(u^*, u^*) = (1, u^*)$ we can compute $a_{s,\rho}(u^*, u^*)$ and compare it with $(1, u^*) = \int_\Omega u^* dx$, whose value is explicitly computable

$$\int_{B_R(x_0)} u^* dx = \begin{cases} c_{1,s} \frac{\sqrt{\pi} R^{2s+1} \Gamma(s+1)}{\Gamma(s+3/2)}, & \text{for } d = 1, \\ c_{2,s} \frac{\pi R^{2s+2}}{s+1}, & \text{for } d = 2. \end{cases} \quad (5.14)$$

In Figure 5.2 we see that the observed orders of convergence for different values of s seem to match the ones contained in the estimate (5.11), in both one and two dimensions.

In Figures 5.3 and 5.4 we collect the results of computing the approximated solution $u_{h,\rho}$ with a WFEM approach, for different values of h and ρ , respectively in one and two dimensions.

In Figure 5.5 we report the results of doing the same, but using a FEM approach with a standard piecewise linear basis.

Remark 5.6. In one dimension, in the special case of f constant, the entries F_i of the right-hand side in (4.16) can be computed exactly even in the case of WFEM. In fact, if f is constant the computation of F_i in one dimension reduces to integrals of the form

$$\int_a^b \delta(x)^s dx \quad \text{and} \quad \int_a^b \delta(x)^s x dx,$$

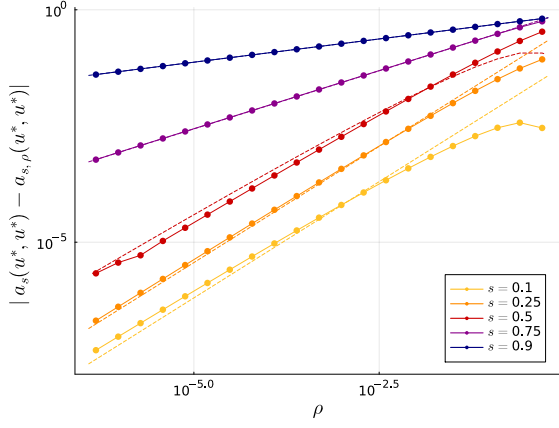
since an element of the basis of V_h has the form $\zeta_i = \delta^s \phi_i$, for $\phi_i \in \text{PL}(\mathcal{T}_h)$.

If, for example, $\Omega = (-1, 1)$, and $\delta(x) = 1 - |x|^p$ (the setting of our numerical experiments), one can explicitly compute the following primitives: for $x \geq 0$

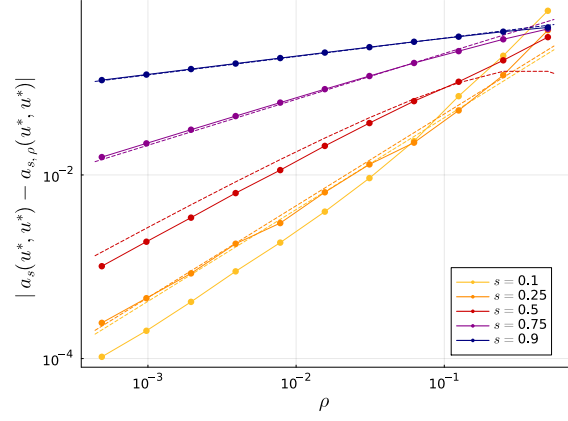
$$\begin{aligned} G_1(x) &= x {}_2F_1\left(\frac{1}{p}, -s; 1 + \frac{1}{p}; x^p\right), & G'_1(x) &= (1 - x^p)^s, \\ G_2(x) &= \frac{x^2}{2} {}_2F_1\left(\frac{2}{p}, -s; 1 + \frac{2}{p}; x^p\right), & G'_2(x) &= x(1 - x^p)^s, \end{aligned}$$

where ${}_2F_1$ is the Gaussian hypergeometric function.

Two main facts can be inferred comparing the results in Figures 5.3, 5.4 and Figure 5.5. On the one hand a significantly smaller value of ρ needs to be employed for WFEM to suppress the error arising from the quadrature of the bilinear form (5.2). This is due to the presence of E_h^2 and $\omega_{a,X}(\rho)$ in the Strang-type estimate (5.6): their value is expected to be worse than a standard finite element method with a piecewise linear basis. As discussed previously, intuitively the choice of $V_h = \delta^s \text{PL}(\mathcal{T}_h)$ as the functional space for the basis functions and the consequent lower regularity affect the way in which the singularity of the kernel in the integral fractional Laplacian is handled by the quadrature approximation. On the other hand, if one is willing to pay the computational cost that comes with using a smaller ρ we clearly observe the gain in digits of accuracy both in one and two dimensions for WFEM, compared to FEM for the same values of h . We recall that the stiffness matrix $A_{s,\rho}$ is a symmetric dense matrix that needs at least half of it to be fully stored in practice. This fact further motivates the possibility of using WFEM to gain higher accuracy for a relatively coarse mesh in h . Finally, we remark that WFEM is more advantageous for smaller values of s , where the benefit of using a basis with lower regularity is very visible compared to FEM.

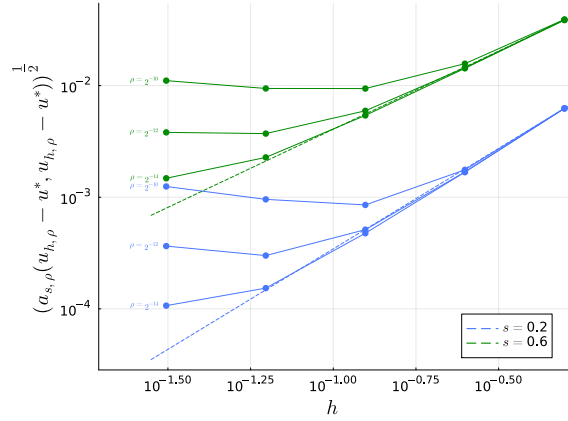
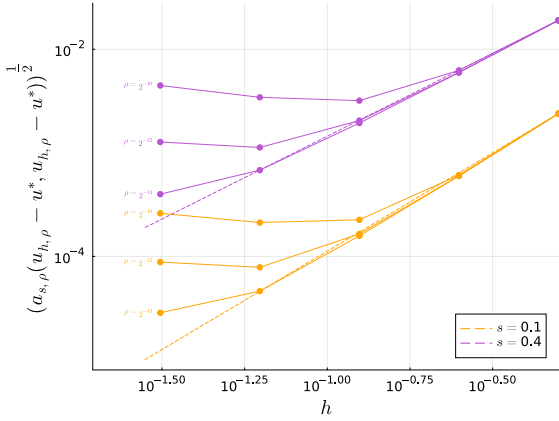


(a) $d = 1$, $\rho = 2^{-n}$ $n = 1, \dots, 21$.



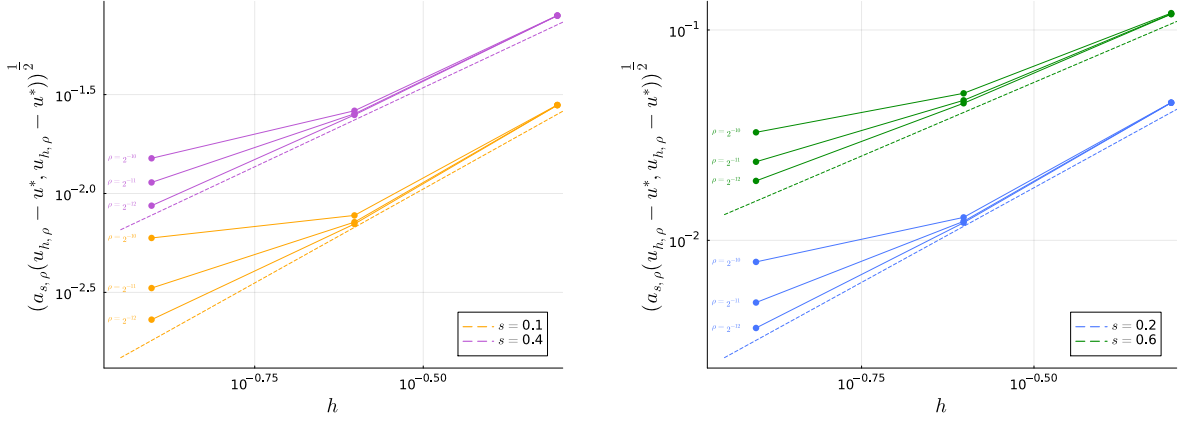
(b) $d = 2$, $\rho = 2^{-n}$ $n = 1, \dots, 11$.

Figure 5.2: Convergence of $a_{s,\rho}$ to a_s in dimension $d = 1, 2$. The simulations were performed for different fractional orders s . The domain is $\Omega = (-1, 1)$ in one dimension and $\Omega = B_1(0)$ in two dimensions, the quadrature points are equally spaced in Ω for different values of ρ . The expected orders of convergence (5.11) are reported as dashed lines.



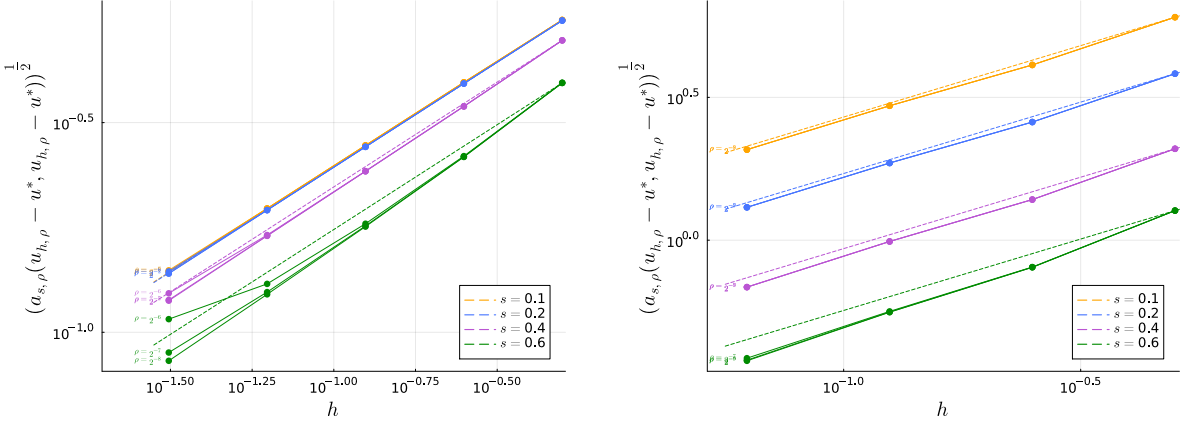
(a) approximate $H^s(\mathbb{R})$ seminorm of the error, $(a_{s,\rho}(u_{h,\rho} - u^*, u_{h,\rho} - u^*))^{1/2}$, dashed lines: Ch^{2-s} . (b) approximate $H^s(\mathbb{R})$ seminorm of the error, $(a_{s,\rho}(u_{h,\rho} - u^*, u_{h,\rho} - u^*))^{1/2}$, dashed lines: Ch^{2-s} .

Figure 5.3: WFEM computational errors and dependence on the mesh size h and the quadrature parameter ρ in dimension $d = 1$. The simulations were performed for different fractional orders s . The computational domain is $\Omega = (-1, 1)$, $\Omega_h = \Omega$. The quadrature points are equally spaced for different values of $\rho = 2^{-10}, 2^{-12}, 2^{-14}$. The value of ε_ρ is set to ρ and $R = +\infty$.



(a) approximate $H^s(\mathbb{R}^2)$ seminorm of the error, $(a_{s,\rho}(u_{h,\rho} - u^*, u_{h,\rho} - u^*))^{1/2}$, dashed lines: Ch^{2-s} . (b) approximate $H^s(\mathbb{R}^2)$ seminorm of the error, $(a_{s,\rho}(u_{h,\rho} - u^*, u_{h,\rho} - u^*))^{1/2}$, dashed lines: Ch^{2-s} .

Figure 5.4: WFEM computational errors and dependence on the mesh size h and the quadrature parameter ρ in dimension $d = 2$. The simulations were performed for different fractional orders s . The computational domain is $\Omega = B_1(0) \subset \mathbb{R}^2$, $\Omega_h = (-1, 1)^2$ with a uniform mesh. The quadrature points are equally spaced for different values of $\rho = 2^{-10}, 2^{-11}, 2^{-12}$.



(a) approximate $H^s(\mathbb{R})$ seminorm of the error, $(a_{s,\rho}(u_{h,\rho} - u^*, u_{h,\rho} - u^*))^{1/2}$, dashed lines: $Ch^{1/2}$, $\rho = 2^{-6}, 2^{-7}, 2^{-8}$. (b) approximate $H^s(\mathbb{R}^2)$ seminorm of the error, $(a_{s,\rho}(u_{h,\rho} - u^*, u_{h,\rho} - u^*))^{1/2}$, dashed lines: $Ch^{1/2}$, $\rho = 2^{-7}, 2^{-8}, 2^{-9}$.

Figure 5.5: FEM computational errors and dependence on the mesh size h and the quadrature parameter ρ . The simulations were performed for different fractional orders s . The computational domains are respectively $\Omega = (-1, 1)$ in one dimension and a Lipschitz approximation of $\Omega = B_1(0) \subset \mathbb{R}^2$, consisting of triangles, in two dimensions, the quadrature points are equally spaced with different values of ρ . The value of ε_ρ is set to ρ and $R = +\infty$. Dashed lines: $g(h) = Ch^{1/2}$

Domani è un altro giorno, si vedrà.

Ornella Vanoni (1934–2025), “Domani È Un Altro Giorno”

Conclusion

We conclude by summarising the work what we have presented and highlighting some open problems related to our analysis and future directions for research, some of which have been already mentioned in passing in different chapters of the thesis.

We have developed and studied numerical methods based on finite elements for nonlinear PDEs that involve the fractional Laplacian operator. The main class of problems that we have considered are diffusion equations of porous medium type, where the pressure is defined through the fractional Laplacian (1.2) and then generalised to fractional powers of other elliptic operators (3.16). For models of this type we have considered the spectral definition of these fractional operators and we have developed finite element schemes accordingly. In our work, all the diffusion models had a parabolic regularisation term that was required in order to guarantee uniform control of the relevant norms of the numerical approximations. Using these uniform bounds we performed a rigorous passage to the limit in the space and time discretizations, using both intrinsic properties of the equations and techniques for nonlinear PDEs. For the model (1.2) it was also possible to prove exponential decay of the energy and the exponential decay to the constant steady state, while the structure of the generalised model (3.16) did not allow us to obtain similar results, even though we believe that similar properties hold.

From a theoretical perspective there are two main open problems related to our finite element scheme and they are the use of a regularisation parameter and the ordered passage to the limit (first in space with $h \rightarrow 0$ and then in time $\Delta t \rightarrow 0$). More precisely, the use of the cut-off parameter $L > 0$ from above served the purpose of having uniform estimates in h without knowing a bound on the L^∞ norm of the solution; such a result was provable only using the L^∞ contractivity of the heat semigroup associated to the fractional elliptic operators that we have considered. We believe that a bound on the $L^\infty(\Omega)$ norm of the fully discrete solution could be proved; computational evidence was given in Chapter 2 with all the numerical simulations enforcing this intuition. If one could prove a uniform bound on the $L^\infty(\Omega)$ norm of the fully discrete numerical solution we could drop the use of the parameter L and then potentially develop a simultaneous passage to the limit as h and Δt tend to zero.

In Chapter 2 we discussed another PDE, analogous of (1.2): the fractional Keller–Segel model (2.31). In contrast with the other models, the equation is an aggregation-diffusion equation that models a competing effect between standard diffusion and nonlocal aggregation, induced by a

change of sign in the potential term of (1.2). We studied this more complex problem mainly from a scientific computing perspective, presenting only a proof of finite-in-time blow-up for a weak solution of the problem. From an analytical point of view, an interesting direction of work for this equation would be to try to design a finite element scheme similar to the one that was developed in Chapter 1 to prove *local-in-time* existence of a solution. Ideally, the strategy to develop such a scheme would be to use a varying time step $\Delta t^{(n)} := t_n - t_{n-1}$ that decreases in order to have uniform control of spatial norms of the numerical solution and prove spatial convergence as $h \rightarrow 0$ under this constraint. Eventually we would expect to have a finite quantity $T^\dagger := \sum_{n=1}^{\infty} \Delta t^{(n)} < \infty$. This time $T^\dagger$ would then be an approximation of the blow-up time of the solution. Any dependence of $T^\dagger$ with respect to the mass of the solution, its initial concentration and the fractional order s would be interesting features that have not been studied before, theoretically or computationally. Moreover, the accuracy of the numerically predicted blow-up time $T^\dagger$ could then be studied using the scientific computing tools that we have tested in Chapter 2.

With respect to the algorithm described in Chapter 2, we have used minimax as algorithm to compute the rational approximation that was then used for computing the finite element approximation of the inverse fractional Laplacian. However, over the past decades, many algorithms were developed for the computation of rational approximations of functions and their application to problems in numerical linear algebra. Exploring the use of alternative rational approximation algorithms for the type of evolution problems considered here constitutes an interesting direction for future research.

As regards the generalised models (3.16), we had to restrict the fractional order to $s \in (1/2, 1)$. The reason was to have uniform control of the $H^1(\Omega)$ seminorm of the potential because this was not attainable directly from the bilinear form (3.11) for a general elliptic operator, as we did for the fractional Laplacian. Finding a way to weaken this hypothesis and obtain the full range $(0, 1)$ for the fractional order is an open problem that would require technical results for the regularity of the potential. Moreover proving exponential decay to nontrivial steady states and exponential decay of the energy is a complex task that could require a different approach. Nevertheless, these facts are substantiated by the numerical experiments that we presented in Chapter 3.

Going beyond the models that we have presented in the current thesis, there are equations which are direct, yet highly challenging, generalisations of the porous medium equation with a fractional pressure and a parabolic regularisation that we have considered. These models are obtained by changing the standard diffusion term. In other words, we could ask which types of numerical schemes are applicable to PDEs where the simple parabolic regularisation term is replaced by nonlinear diffusion or also by fractional diffusion. For example, problems of the type

$$\frac{\partial \rho}{\partial t} = \Delta \rho^m + \nabla \cdot (\rho \nabla c), \quad \pm (-\Delta)^s c = \rho \quad (5.15)$$

or

$$\frac{\partial \rho}{\partial t} = -(-\Delta)^\sigma \rho + \nabla \cdot (\rho \nabla c), \quad \pm(-\Delta)^s c = \rho, \quad (5.16)$$

open a new horizon for further work. Aggregation-diffusion equations with nonlocal interaction kernels, related to (5.15), have been studied in the foundational work [63] and then investigated further in [34, 66], computing long time asymptotics; we refer also to [61] for a more extensive survey of the topic. The model (5.16) has been studied in the case of an attractive potential in [33] for $s = 1$ and in [31, 130] in the more general case $0 < \sigma < 1$ and $0 < s < 1$, mainly focusing on the blow-up of the solution and its dependence on s and σ . The development of numerical methods on a bounded domain for this type of problem constitutes a largely unexplored field, that could offer significant potential in terms of modelling.

With regards to the finite element method with a weighted basis that we have analyzed in Chapter 4 there are several questions for future work. In the first place, since the regularity of u/δ^s can be arbitrarily high (see (4.12)), provided that f and Ω are regular enough, a possibility would be to use higher order elements to achieve higher order convergence rates. A close inspection of the proofs suggests that for a basis of elements of degree $k \in \mathbb{N}$, the order of convergence in the s -Sobolev norm could be h^{k+1-s} . The approach that we have discussed relies on the observation that for solutions of (4.1) the quotient u/δ^s is highly regular. This feature also appears in problems where the fractional Laplacian is replaced by more general nonlocal operators of the form

$$L\phi(y) = \text{P.V.} \int_{\mathbb{R}^d} (\phi(x) - \phi(y)) K(x - y) \, dx,$$

under suitable structural conditions on the kernel K (see [1, 155, 156, 157]). Consequently, weighted finite element methods, such as the one proposed here, are naturally extendable to this broader class of operators.

Finally, another interesting family of problems is

$$(-\Delta)^s u(x) + V(x)u(x) = f(x),$$

where the singularity of the potential V at the boundary may alter the boundary behaviour of u . On the one hand, for $s > 1/2$ if we consider the so-called “killing” potential

$$\kappa(x) = C_{d,s} \int_{\mathbb{R}^d \setminus \Omega} |x - y|^{-d-2s} \, dy \asymp d_\Omega(x)^{-2s},$$

where the symbol $\asymp$ denotes two-sided comparability up to a positive multiplicative constant, then $V(x) = -\kappa(x)$ gives the so-called Censored Fractional Laplacian $(-\Delta)_{\text{CFL}}^s := (-\Delta)^s + V$. In this setting it is known that for f nonnegative and bounded we have $u \asymp d_\Omega^{2s-1}$. The regularity theory for u/d_Ω^{2s-1} is available in [100], and the natural weighted basis for a finite element theory similar to the one presented in this thesis is $\delta^{2s-1} \text{PL}(\mathcal{T}_h)$. On the other hand, for any $\varepsilon \in (0, s)$

we can find $C(\varepsilon) > 0$ such that, if $V \geq C(\varepsilon)d_{\Omega}^{-2s}$, then $|u| \leq Cd_{\Omega}^{s+\varepsilon}$ near $\partial\Omega$ (see [89]). In this setting it would be interesting to see whether using a suitably weighted basis results in improvements.



The spectral fractional Laplacian and fractional elliptic operators

We report here certain technical results related to the spectral fractional Neumann Laplacian (1.5) and to general fractional elliptic operators (3.14) paired with a Neumann boundary condition. These results are of relevance for our analysis and constitute a useful set of properties for further problems.

Let $\mathcal{L}$ be an operator such as the one described in Chapter 3, more precisely as in (3.5) $\mathcal{L}u = -\operatorname{div}(A(x)\nabla u) + Q(x)u$, with $-\operatorname{div}(A(x)\nabla(\cdot))$ as the principal part of the operator. Let $\mathcal{L}_N$ be the operator paired with a Neumann boundary condition, let $\mathcal{L}_N^s$ its fractional power defined in (3.14) and $\mathcal{H}_\diamond^s(\Omega)$ the fractional Sobolev space associated to it and defined in (3.15). For a bounded open Lipschitz domain $\Omega \subset \mathbb{R}^d$, $s \in (0, 1)$, and $f \in \mathcal{H}_\diamond^{-s}(\Omega)$, consider the following fractional equation with a Neumann boundary condition:

$$\mathcal{L}_N^s u = f \quad \text{in } \Omega, \quad A(x)\nabla u \cdot n = 0 \quad \text{on } \partial\Omega. \quad (\text{A.1})$$

By a *weak solution* to (A.1) we mean a function $u \in \mathcal{H}_\diamond^s(\Omega)$, $s \in (0, 1)$, such that

$$\int_{\Omega} (\mathcal{L}_N^{s/2} u(x)) (\mathcal{L}_N^{s/2} v(x)) \, dx = \langle f, v \rangle \quad \forall v \in \mathcal{H}_\diamond^s(\Omega),$$

where $\langle \cdot, \cdot \rangle$ denotes the duality pairing between $\mathcal{H}_\diamond^{-s}(\Omega)$ and $\mathcal{H}_\diamond^s(\Omega)$, with $\mathcal{H}_\diamond^s(\Omega) \hookrightarrow \mathcal{H}^0(\Omega) \equiv \mathcal{H}^0(\Omega)' \hookrightarrow \mathcal{H}_\diamond^{-s}(\Omega)$ and $\mathcal{H}_\diamond^0(\Omega) = L_\diamond^2(\Omega)$, where $L_\diamond^2(\Omega)$ stands for the space defined in (3.12). In particular if $f \in L_\diamond^2(\Omega)$, then $\langle f, v \rangle = (f, v)$ for all $v \in \mathcal{H}_\diamond^s(\Omega)$, $s \in [0, 1)$.

In the case $\mathcal{L} = -\Delta$, $\mathcal{H}_\diamond^s(\Omega) = \mathbb{H}_*^s(\Omega)$ and problem (A.1) reduces to a fractional Poisson equation involving the Neumann Laplacian:

$$(-\Delta_N)^s u = f \quad \text{in } \Omega, \quad (\text{A.2})$$

with $f \in \mathbb{H}_*^{-s}(\Omega)$. By a *weak solution* to (A.2) we mean a function $u \in \mathbb{H}_*^s(\Omega)$, $s \in (0, 1)$, such that

$$\int_{\Omega} ((-\Delta_N)^{s/2} u(x)) ((-\Delta_N)^{s/2} v(x)) \, dx = \langle f, v \rangle \quad \forall v \in \mathbb{H}_*^s(\Omega),$$

where $\langle \cdot, \cdot \rangle$ denotes the duality pairing between $\mathbb{H}_*^{-s}(\Omega)$ and $\mathbb{H}_*^s(\Omega)$.

Theorem A.1 (Existence and uniqueness of a weak solution). *Suppose that $\Omega \subset \mathbb{R}^d$ is a bounded open Lipschitz domain, $s \in (0, 1)$, and $f \in \mathcal{H}_{\diamond}^{-s}(\Omega)$. Then, the boundary-value problem (A.1) has a unique weak solution $u \in \mathcal{H}_{\diamond}^s(\Omega)$, and*

$$\|u\|_{\mathcal{H}_{\diamond}^s(\Omega)} \leq \|f\|_{\mathcal{H}_{\diamond}^{-s}(\Omega)}. \quad (\text{A.3})$$

Proof. The existence of a unique weak solution $u \in \mathcal{H}_{\diamond}^s(\Omega)$ is a direct consequence of the Lax–Milgram lemma applied to the variational problem: find $u \in \mathcal{H}_{\diamond}^s(\Omega)$ such that $a(u, v) = \ell(v)$ for all $v \in \mathcal{H}_{\diamond}^s(\Omega)$, with the bilinear form

$$a(w, v) := \int_{\Omega} (\mathcal{L}_N^{s/2} w(x)) (\mathcal{L}_N^{s/2} v(x)) \, dx, \quad w, v \in \mathcal{H}_{\diamond}^s(\Omega),$$

and the linear functional $\ell(v) := \langle f, v \rangle$, $v \in \mathcal{H}_{\diamond}^s(\Omega)$. The stated stability inequality follows by noting that

$$\|u\|_{\mathcal{H}_{\diamond}^s(\Omega)}^2 = a(u, u) = \langle f, u \rangle \leq \|f\|_{\mathcal{H}_{\diamond}^{-s}(\Omega)} \|u\|_{\mathcal{H}_{\diamond}^s(\Omega)}.$$

This completes the proof of the theorem. $\square$

We note in passing that the following function space interpolation inequality holds.

Lemma A.2. *Let $\Omega \subset \mathbb{R}^d$ be a bounded open Lipschitz domain, $s \in (0, 1)$, and $u \in \mathcal{H}_{\diamond}^1(\Omega)$. Then,*

$$\|u\|_{\mathcal{H}_{\diamond}^s(\Omega)} \leq \|u\|_{L^2(\Omega)}^{1-s} \|u\|_{\mathcal{H}^1(\Omega)}^s.$$

Proof. The assertion of the lemma follows by applying Hölder's inequality and the definition (3.15). Indeed, without loss of generality, let the positive eigenvalues corresponding to $\mathcal{L}_N$ be μ_k , $k = 1, 2, \dots$, we have for $\theta \in (0, 1)$ that

$$\|u\|_{\mathcal{H}_{\diamond}^s(\Omega)}^2 = \sum_{k=1}^{\infty} \mu_k^s u_k^2 = \sum_{k=1}^{\infty} |u_k|^{\theta} \mu_k^s |u_k|^{2-\theta} \leq \left(\sum_{k=1}^{\infty} |u_k|^{\theta p} \right)^{\frac{1}{p}} \left(\sum_{k=1}^{\infty} \mu_k^{sq} |u_k|^{(2-\theta)q} \right)^{\frac{1}{q}},$$

for $p, q \in (1, \infty)$ such that $\frac{1}{p} + \frac{1}{q} = 1$. The stated inequality then follows by taking $p = \frac{2}{\theta}$, $q = \frac{2}{2-\theta}$ and $\theta = 2(1-s)$, whereby $\theta p = 2$, $sq = 1$, $(2-\theta)q = 2$, $1/p = \theta/2 = 1-s$, and $1/q = s$. $\square$

Lemma A.3. Suppose that $\Omega \subset \mathbb{R}^d$ is a bounded open Lipschitz domain, $s \in (0, 1)$. Assume $\mathcal{L}_N$ is such that $Q = 0$ a.e. in Ω . Let $u \in \mathcal{H}_\diamond^s(\Omega)$. If $u \in H^1(\Omega)$, then the following pair of inequalities holds for positive constants $C_1, C_2 > 0$ independent of u :

$$C_1 \|u\|_{L^2(\Omega)} \leq \|u\|_{\mathcal{H}_\diamond^s(\Omega)} \leq C_2 |u|_{H^1(\Omega)}. \quad (\text{A.4})$$

In particular, the above inequalities imply that a Poincaré-type inequality holds for functions in $\mathcal{H}_\diamond^s(\Omega)$.

Proof. Let us first recall that $\|\cdot\|_{\mathcal{H}_\diamond^1(\Omega)}$ and $|\cdot|_{H^1(\Omega)}$ are equivalent on $\mathcal{H}_\diamond^s(\Omega)$ (see the discussion after (3.15)). Let φ_k , $k = 1, 2, \dots$, denote the eigenfunctions of the operator $\mathcal{L}_N$ corresponding to the positive eigenvalues μ_k , $k = 1, 2, \dots$, where μ_1 is the smallest positive eigenvalue. We have immediately that

$$\mu_1^s \|u\|_{L^2(\Omega)}^2 \leq \|u\|_{\mathcal{H}_\diamond^s(\Omega)}^2,$$

proving the first inequality in (A.4). Since $0 < s < 1$ we also have

$$\|u\|_{\mathcal{H}_\diamond^s(\Omega)}^2 = \sum_{k=1}^{\infty} \mu_k^s u_k^2 = \sum_{k=1}^{\infty} \mu_k^{s-1} \mu_k u_k^2 \leq \mu_1^{s-1} \sum_{k=1}^{\infty} \mu_k u_k^2 = \mu_1^{s-1} \|u\|_{\mathcal{H}_\diamond^1(\Omega)}^2.$$

This, together with the equivalence of $\|\cdot\|_{\mathcal{H}_\diamond^1(\Omega)}$ and $|\cdot|_{H^1(\Omega)}$, completes the proof of (A.4). $\square$

The following result has been proved in [57, Lemma 7.1] for the case in which $\mathcal{L}u = \operatorname{div}(A(x)\nabla u)$.

Proposition A.4. Assume $\mathcal{L}_N$ is such that $Q = 0$ a.e. in Ω . Let $u \in \mathcal{H}_\diamond^s(\Omega)$. If $u \in H^s(\Omega)$, then the following norm equivalence holds:

$$\|u\|_{\mathcal{H}_\diamond^s(\Omega)} \sim |u|_{H^s(\Omega)}.$$

Remark A.5. For the Neumann fractional Laplacian, Proposition A.4 means that for any $s \in (0, 1)$, a function u belongs to $\mathbb{H}_*^s(\Omega)$ if and only if $u \in H^s(\Omega)$ and $\int_\Omega u \, dx = 0$; furthermore, the norm $\|\cdot\|_{\mathbb{H}_*^s(\Omega)}$ is equivalent to the seminorm $|\cdot|_{H^s(\Omega)}$, which is a norm on $H_*^s(\Omega)$. In fact, any function u belonging to $\mathbb{H}_*^s(\Omega)$, $s \in (0, 1)$, satisfies $\int_\Omega u \, dx = 0$.

An important result that we rely on throughout our analysis is the following H^1 norm stability of the problem (A.1).

Lemma A.6. Suppose that $\Omega \subset \mathbb{R}^d$ is a bounded open Lipschitz domain, $s \in (0, 1)$, and $f \in H^1(\Omega) \cap L_\diamond^2(\Omega)$. Assume $\mathcal{L}_N$ is such that $Q = 0$ a.e. in Ω . Suppose further that $u \in \mathcal{H}_\diamond^s(\Omega)$ is the unique weak solution of (A.1). Then $u \in H^1(\Omega)$ and there exists a positive constant C such that

$$\|\nabla u\|_{L^2(\Omega)} \leq C \mu_1^{-\frac{s}{2}} \|\nabla f\|_{L^2(\Omega)}, \quad (\text{A.5})$$

where μ_1 is the smallest positive eigenvalue of the operator $\mathcal{L}_N$ on Ω . Moreover, if $s \in [1/2, 1)$, then also

$$\|\nabla u\|_{L^2(\Omega)} \leq C \mu_1^{\frac{1-2s}{2}} \|f\|_{L^2(\Omega)}, \quad (\text{A.6})$$

for a positive constant $C > 0$.

Proof. Let φ_k , $k = 1, 2, \dots$, denote the eigenfunctions of the operator $\mathcal{L}$ corresponding to the positive eigenvalues μ_k , $k = 1, 2, \dots$, where μ_1 is the smallest positive eigenvalue. As $\{\varphi_k\}_{k \geq 1}$ is a complete orthonormal system in $L^2_\diamond(\Omega)$ and $f \in H^1_\diamond(\Omega) \cap L^2_\diamond(\Omega) \subset L^2_\diamond(\Omega)$, it follows that

$$f(x) = \sum_{k=1}^{\infty} f_k \varphi_k(x), \quad \text{with } f_k := \int_{\Omega} f(x) \varphi_k(x) \, dx,$$

with the convergence of the series understood to be in the norm of $L^2(\Omega)$; i.e., the M -th partial sum

$$f^M(x) := \sum_{k=1}^M f_k \varphi_k(x), \quad x \in \Omega,$$

converges to f strongly in the norm of $L^2(\Omega)$. Similarly, because $u \in \mathcal{H}^s_\diamond(\Omega) \subset L^2_\diamond(\Omega)$, we have that

$$u(x) = \sum_{k=1}^{\infty} u_k \varphi_k(x), \quad \text{with } u_k := \int_{\Omega} u(x) \varphi_k(x) \, dx,$$

and the M -th partial sum

$$u^M(x) := \sum_{k=1}^M u_k \varphi_k(x), \quad x \in \Omega,$$

converges to u strongly in the norm of $L^2(\Omega)$. Because u is the unique weak solution of (A.1), it follows by taking $v = \varphi_k$ as test function in the weak formulation that $u_k := \mu_k^{-s} f_k$, $k = 1, 2, \dots$. Furthermore,

$$\begin{aligned} (\mathcal{L}^{1/2} u^M, \mathcal{L}^{1/2} u^M) &= \left(\sum_{k=1}^M u_k \mathcal{L}^{1/2} \varphi_k, \sum_{\ell=1}^M u_\ell \mathcal{L}^{1/2} \varphi_\ell \right) = \sum_{k=1}^M \sum_{\ell=1}^M u_k u_\ell (\mathcal{L}^{1/2} \varphi_k, \mathcal{L}^{1/2} \varphi_\ell) \\ &= \sum_{k=1}^M \sum_{\ell=1}^M u_k u_\ell (\mathcal{L} \varphi_k, \varphi_\ell) = \sum_{k=1}^M \sum_{\ell=1}^M \mu_k u_k u_\ell (\varphi_k, \varphi_\ell) = \sum_{k=1}^M \sum_{\ell=1}^M \mu_k u_k u_\ell \delta_{k,\ell} \\ &= \sum_{k=1}^M \mu_k u_k^2 = \sum_{k=1}^M (\mu_k)^{1-2s} f_k^2 \leq \mu_1^{-s} \sum_{k=1}^M (\mu_k)^{1-s} f_k^2 \end{aligned} \quad (\text{A.7})$$

$$\leq \mu_1^{-s} \sum_{k=1}^{\infty} (\mu_k)^{1-s} f_k^2 = \mu_1^{-s} \|f\|_{\mathcal{H}^{1-s}_\diamond(\Omega)}^2 \quad \forall M \geq 1. \quad (\text{A.8})$$

Since $f \in H^1(\Omega) \cap L^2_\diamond(\Omega)$, by Lemma A.3 we immediately have that there exists a constant $C > 0$ such that

$$(\mathcal{L}^{1/2} u^M, \mathcal{L}^{1/2} u^M) \leq C \mu_1^{-s} \|\nabla f\|_{L^2(\Omega)}^2 \quad \forall M \geq 1. \quad (\text{A.9})$$

We notice now that, using the explicit expression of the operator $\mathcal{L}_N$ (3.5), we have

$$(\mathcal{L}^{1/2}w, \mathcal{L}^{1/2}w) = (\mathcal{L}w, w) = \int_{\Omega} (A(x)\nabla w, \nabla w) dx + \int_{\Omega} Q(x)w^2 dx \geq \Lambda_1 \|\nabla w\|_{L^2(\Omega)}^2 \quad (\text{A.10})$$

and thus

$$\|\nabla u^M\|_{L^2(\Omega)}^2 \leq C\mu_1^{-s} \|\nabla f\|_{L^2(\Omega)}^2 \quad \forall M \geq 1. \quad (\text{A.11})$$

Using an analogous calculation to the one in (A.8), together with (A.10), for any positive integers M and N such that $M > N$ we have that

$$\|\nabla u^M - \nabla u^N\|_{L^2(\Omega)}^2 \leq \mu_1^{-s} \sum_{k=N+1}^M (\mu_k)^{1-s} f_k^2.$$

Because the infinite series appearing in the last line of (A.8) is convergent, it then follows that for any $\varepsilon > 0$ there exist positive integers M and N , with $M > N$, such that

$$\|\nabla u^M - \nabla u^N\|_{L^2(\Omega)}^2 \leq \mu_1^{-s} \sum_{k=N+1}^M (\mu_k)^{1-s} f_k^2 < \varepsilon,$$

i.e., $(\nabla u^M)_{M \geq 1}$ is a Cauchy sequence in the Hilbert space $L^2(\Omega; \mathbb{R}^d)$; therefore ∇u^M converges (strongly in the norm of $L^2(\Omega; \mathbb{R}^d)$) to an element of $L^2(\Omega; \mathbb{R}^d)$. As u^M converges to $u \in L^2(\Omega)$ strongly in the norm of $L^2(\Omega)$, by the uniqueness of the limit, ∇u^M must converge to ∇u in $L^2(\Omega; \mathbb{R}^d)$. Therefore,

$$\lim_{M \rightarrow \infty} \|\nabla u^M\|_{L^2(\Omega)}^2 = \|\nabla u\|_{L^2(\Omega)}^2.$$

With this information we now return to (A.11) and pass to the limit $M \rightarrow \infty$ on the left-hand side of the inequality to deduce the desired inequality (A.5).

Inequality (A.6) can be proved by following the same argument, but also using in (A.7) and the assumed constraint that $s \in [1/2, 1)$, which implies that $1 - 2s \leq 0$; therefore,

$$\|\nabla u^M\|_{L^2(\Omega)}^2 \leq C\mu_1^{1-2s} \|f\|_{L^2(\Omega)}^2 \quad \forall M \geq 1.$$

The desired inequality then follows by passing to the limit $M \rightarrow \infty$. This completes the proof. $\square$

In our context another useful result is a type of Sobolev–Poincaré inequality. In [125] it was shown that, for a bounded open John domain $\Omega \subset \mathbb{R}^d$, the following inequality holds for $s, \tau \in (0, 1)$, $p < d/s$ and $1 < p \leq q \leq \frac{dp}{d-sp}$:

$$\|u - \bar{u}\|_{L^q(\Omega)} \leq C \left(\int_{\Omega} \int_{\Omega \cap B(x, \tau \text{dist}(x, \partial\Omega))} \frac{|u(x) - u(y)|^p}{|x - y|^{d+sp}} dy dx \right)^{\frac{1}{p}}. \quad (\text{A.12})$$

The seminorm appearing on the right-hand side of (A.12) is weaker than the usual Gagliardo–Slobodetskii seminorm of the fractional-order Sobolev space $W^{s,p}(\Omega)$,

$$\left(\int_{\Omega} \int_{\Omega} \frac{|u(x) - u(y)|^p}{|x - y|^{d+sp}} dx dy \right)^{\frac{1}{p}}.$$

Indeed, the two seminorms induce different fractional order Sobolev spaces, which coincide in the case of a bounded open Lipschitz domain, as was shown in [96]. Thus, in the case of a Lipschitz domain Ω , as is the case in the setting under consideration in this thesis, and for $p = q = 2$, we have the following fractional Poincaré inequality for $s \in (0, 1)$:

$$\|u - \bar{u}\|_{L^2(\Omega)} \leq C|u|_{H^s(\Omega)}, \quad (\text{A.13a})$$

where C is a positive constant, independent of u . Therefore, in particular,

$$\|u\|_{L_*^2(\Omega)} \leq C|u|_{H_*^s(\Omega)}. \quad (\text{A.13b})$$

We notice how an analogous inequality holds in general for functions $u \in \mathcal{H}_\diamond^s(\Omega)$ and $s \in (0, 1)$: one has that

$$\|u\|_{L_\diamond^2(\Omega)} \leq \mu_1^{-s/2} \|u\|_{\mathcal{H}_\diamond^s(\Omega)}. \quad (\text{A.13c})$$

This inequality, in conjunction with Theorem A.1, ensures the $L_\diamond^2(\Omega)$ norm stability of the weak solution to the fractional Poisson equation based on the spectral definition of $\mathcal{L}_N$, for $f \in L_\diamond^2(\Omega)$.

We now prove some auxiliary results, which concern the case when the right-hand side datum of equation (A.2) has $L^\infty(\Omega)$ regularity or $W^{1,\infty}(\Omega)$ regularity. Let us denote respectively by $L_*^\infty(\Omega)$ and $W_*^{1,\infty}(\Omega)$ the spaces of functions in $L^\infty(\Omega)$ and $W^{1,\infty}(\Omega)$ with zero integral average over Ω .

For the Neumann spectral fractional Laplacian, it is possible to prove an additional result, which gives a further expression for its inverse.

Lemma A.7. *Suppose that $\Omega \subset \mathbb{R}^d$ is a bounded open Lipschitz domain, $s \in (0, 1)$, and $f \in L_*^\infty(\Omega)$. Then, we have that*

$$(-\Delta_N)^{-s} f \simeq C_{\Omega,s,d} \int_\Omega \frac{1}{|x-y|^{d-2s}} f(y) \, dy, \quad (\text{A.14})$$

for a positive constant $C_{\Omega,s,d}$ depending only on Ω, s and d .

Proof. Since $L_*^\infty(\Omega) \subset L_*^2(\Omega) \subset \mathbb{H}_*^{-s}(\Omega)$, we have that

$$(-\Delta_N)^{-s} f = \sum_{k=1}^{\infty} \lambda_k^{-s} f_k \psi_k, \quad \text{where } f_k = \int_\Omega f \psi_k \, dx. \quad (\text{A.15})$$

By noting that for $\lambda > 0$ and $s \in (0, 1)$,

$$\lambda^{-s} = \frac{1}{\Gamma(s)} \int_0^\infty e^{-t\lambda} \frac{1}{t^{1-s}} \, dt,$$

and inserting this in (A.15), we get that

$$\begin{aligned} (-\Delta_N)^{-s} f &= \frac{1}{\Gamma(s)} \int_0^\infty \sum_{k=1}^{\infty} e^{-t\lambda_k} f_k \psi_k \frac{1}{t^{1-s}} \, dt = \frac{1}{\Gamma(s)} \int_0^\infty \frac{e^{t\Delta_N} f}{t^{1-s}} \, dt \\ &= \frac{1}{\Gamma(s)} \int_0^\infty \int_\Omega W_t(x, y) \frac{1}{t^{1-s}} f(y) \, dy \, dt, \end{aligned} \quad (\text{A.16})$$

where $\{e^{t\Delta_N}\}_{t>0}$ stands for the heat semigroup associated with Δ_N , i.e. $e^{t\Delta_N}u$ solves problem (14) and $W_t(x, y)$ is the distributional heat kernel for $-\Delta$ subject to a homogeneous Neumann boundary condition on $\partial\Omega$.

In [57, Section 7, end of p.804 combined with eq. (2.16)] it has been shown that the fundamental solution of $(-\Delta_N)^s$ verifies the interior estimate

$$\frac{1}{\Gamma(s)} \int_0^\infty W_t(x, y) \frac{1}{t^{1-s}} dt \simeq C_{\Omega, d, s} \frac{1}{|x - y|^{d-2s}}.$$

This, together with expression (A.16), gives us the desired result. $\square$

Corollary A.8. *Suppose that $\Omega \subset \mathbb{R}^d$ is a bounded open Lipschitz domain, $s \in (0, 1)$, and $f \in L_*^\infty(\Omega)$. Let $u \in \mathbb{H}_*^s(\Omega)$ be the unique solution of (A.2). Then $u \in L^\infty(\Omega)$ and*

$$\|u\|_{L^\infty(\Omega)} \leq K_{\Omega, s, d} \|f\|_{L^\infty(\Omega)}, \quad (\text{A.17})$$

for a positive constant $K_{\Omega, s, d}$, depending only on Ω, s and d .

Proof. The proof is a direct consequence of (A.14) and the fact that the function $1/|z|^{d-2s}$ is integrable for $s \in (0, 1)$ over any bounded ball in $\mathbb{R}^d$. $\square$

The following result is an extension to the fractional order setting of a result by Maz'ya [141], concerning the boundedness of the gradient of the solution to the Neumann Laplace problem in a convex domain.

Lemma A.9. *Suppose that $\Omega \subset \mathbb{R}^d$ is a bounded open Lipschitz convex domain, $s \in (1/2, 1)$, and $f \in L_*^\infty(\Omega)$. Let $u \in \mathbb{H}_*^s(\Omega)$ be the unique solution of (A.2). Then, $u \in W_*^{1, \infty}(\Omega)$ and*

$$\|u\|_{W^{1, \infty}(\Omega)} \leq C \|f\|_{L^\infty(\Omega)},$$

for a positive constant $C > 0$.

Proof. By Lemma A.8 we have in the first place that $u \in L^\infty(\Omega)$, with the $L^\infty(\Omega)$ stability bound (A.17).

Let us now prove that $u \in W^{1, \infty}(\Omega)$. We start from expression (A.16) and we use the following inequality for the gradient of the heat kernel:

$$|\nabla_x W_t(x, y)| \leq C_1 \frac{1}{t^{\frac{d+1}{2}}} e^{-|x-y|^2/(C_2 t)}, \quad x, y \in \Omega, \quad t > 0;$$

this inequality is known to hold in bounded open convex domains (cf. [175, Lemma 3.1] or [174, Theorem 1.2]) for positive constants C_1 and C_2 . We then have the following inequality for $x \in \Omega$ and for some positive constant $C > 0$:

$$|\nabla u(x)| \leq C \frac{1}{\Gamma(s)} \int_0^\infty \int_\Omega \frac{1}{t^{\frac{d}{2} + \frac{3}{2} - s}} e^{-|x-y|^2/t} |f(y)| dy dt.$$

By using the change of variable $r = |x - y|^2/t$ in the above equality together with the fact that $f \in L^\infty(\Omega)$, we then have that

$$\begin{aligned} |\nabla u(x)| &\leq C \frac{\|f\|_{L^\infty(\Omega)}}{\Gamma(s)} \int_{\Omega} \frac{1}{|x - y|^{d-2s+1}} \int_0^\infty e^{-r} r^{-\frac{1}{2}-s+\frac{d}{2}} dr dy \\ &= C \frac{\|f\|_{L^\infty(\Omega)}}{\Gamma(s)} \Gamma\left(\frac{d}{2} + \frac{1}{2} - s\right) \int_{\Omega} \frac{1}{|x - y|^{d-2s+1}} dy. \end{aligned}$$

The final assertion of the lemma then follows by noting that the function $1/|z|^{d-2s+1}$ is integrable for $s \in (1/2, 1)$ over any bounded ball in $\mathbb{R}^d$. $\square$

We now present some results concerning the scaling properties of the spectral fractional Laplacian and some useful related inequalities.

Lemma A.10 (Scaling property for the spectral fractional Laplacian). *Let Ω be a bounded Lipschitz star-shaped domain, and for $s \in (0, 1)$ let $(-\Delta_{\mathcal{B}}^\Omega)^s$ be the spectral fractional Laplacian on Ω with boundary condition $\mathcal{B}$, defined in (12). Let $u \in \mathbb{H}_{\mathcal{B}}^s(\Omega)$, where $\mathbb{H}_{\mathcal{B}}^s(\Omega)$ signifies the space $\mathbb{H}^s(\Omega)$ defined in (10) in the case of the Dirichlet Laplacian, and the space $\mathbb{H}^s(\Omega)$ defined in (11) in the case of the Neumann Laplacian. Let $\lambda > 0$, and assume that if $\lambda > 1$ then we have an extension $\bar{u}(x')$ of u to $\lambda\Omega$, with $x' = \lambda x \in \lambda\Omega$ for some $x \in \Omega$, such that $\bar{u} \in \mathbb{H}_{\mathcal{B}}^s(\lambda\Omega)$. Then,*

$$(-\Delta_{\mathcal{B}}^\Omega)^s u_\lambda(x) = \lambda^{2s} [(-\Delta_{\mathcal{B}}^{\lambda\Omega})^s \bar{u}](\lambda x). \quad (\text{A.18})$$

Proof. Let $H_{\mathcal{B}}^1(\Omega)$ denote $H_0^1(\Omega)$ in the case of a homogeneous Dirichlet boundary condition, and $H_*^1(\Omega)$ in the case of a homogeneous Neumann boundary condition. Let us further notice that if $\{\phi_k(x)\}_{k \geq 1}$, $x \in \Omega$ is a set of $L^2(\Omega)$ -orthonormal eigenfunctions of the Laplacian in Ω with boundary condition $\mathcal{B}(\phi_k) = 0$, with corresponding eigenvalues $\{\lambda_k\}_{k \geq 1}$, that is $(\nabla \phi_k, \nabla \phi)_{L^2(\Omega^d)} = \lambda_k (\phi_k, \phi)_{L^2(\Omega)}$ for all $\phi \in H_{\mathcal{B}}^1(\Omega)$, then $\{\phi_k(x'/\lambda)\}_{k \geq 1}$, $x' \in \lambda\Omega$ are a set of eigenfunctions for the Laplacian on $\lambda\Omega$ with corresponding eigenvalues $\{\lambda_k/\lambda^2\}_{k \geq 1}$. This is because for $\phi' \in H_{\mathcal{B}}^1(\lambda\Omega)$, using the change of variables $x' = \lambda x$, one has

$$\begin{aligned} \int_{\lambda\Omega} \nabla_{x'} \phi_k(x'/\lambda) \cdot \nabla_{x'} \phi'(x') dx' &= \lambda^d \int_{\Omega} \nabla_{x'} \phi_k(x) \cdot \nabla_{x'} \phi'(\lambda x) dx \\ &= \frac{\lambda^d}{\lambda^2} \int_{\Omega} \nabla_x \phi_k(x) \cdot \nabla_x \phi'(\lambda x) dx \\ &= \frac{\lambda^d}{\lambda^2} \lambda_k \int_{\Omega} \phi_k(x) \phi'(\lambda x) dx = \frac{\lambda_k}{\lambda^2} \int_{\lambda\Omega} \phi_k(x'/\lambda) \phi'(x') dx'. \end{aligned}$$

If we need $L^2(\lambda\Omega)$ -orthonormal eigenfunctions for the Laplacian on $\lambda\Omega$ we need to choose $\phi'_k(x') := \frac{1}{\lambda^{d/2}} \phi_k(x'/\lambda)$ because $\int_{\lambda\Omega} \phi_k(x'/\lambda) \phi_j(x'/\lambda) dx' = \lambda^d \int_{\Omega} \phi_k(x) \phi_j(x) dx = \lambda^d \delta_{j,k}$.

With these considerations in place we now observe that

$$\begin{aligned}
(-\Delta_{\mathcal{B}}^{\Omega})^s u_{\lambda}(x) &= \sum_{k=1}^{\infty} \lambda_k^s \left(\int_{\Omega} \phi_k(x) \bar{u}(\lambda x) \, dx \right) \phi_k(x) \\
&= \sum_{k=1}^{\infty} \lambda_k^s \left(\int_{\lambda\Omega} \bar{u}(x') \frac{1}{\lambda^{d/2}} \phi_k(x'/\lambda) \, dx' \right) \frac{1}{\lambda^{d/2}} \phi_k(x'/\lambda) \\
&= \lambda^{2s} \sum_{k=1}^{\infty} \left(\frac{\lambda_k}{\lambda^2} \right)^s \left(\int_{\lambda\Omega} \bar{u}(x') \phi'_k(x') \, dx' \right) \phi'_k(x') = \lambda^{2s} [(-\Delta_{\mathcal{B}}^{\lambda\Omega})^s \bar{u}](x'),
\end{aligned}$$

where we have used the change of variable $x' = \lambda x$. $\square$

An inequality analogous to the one stated in the next lemma for the fractional spectral Dirichlet Laplacian is known to hold for the integral representation of the fractional Laplacian in the case of an exterior homogeneous Dirichlet boundary condition (i.e., $u \equiv 0$ on $\mathbb{R}^d \setminus \Omega$) for a bounded star-shaped domain Ω (see [153, 48]).

Lemma A.11 (Pohozaev-type estimate). *Suppose that $\Omega \subset \mathbb{R}^d$ is a bounded Lipschitz star-shaped domain, with $d = 2, 3$, and let $1/2 < s < 1$. Then, for all $u \in H_0^1(\Omega)$ nonnegative with $(-\Delta_D)^s u \in L^2(\Omega)$, we have*

$$\int_{\Omega} (x \cdot \nabla u) (-\Delta_D)^s u \, dx \leq \frac{1}{2} (2s - d) \int_{\Omega} u (-\Delta_D)^s u \, dx. \quad (\text{A.19})$$

Proof. Consider the natural extension of $u \in H_0^1(\Omega)$ to the whole of $\mathbb{R}^d$:

$$\bar{u} := \begin{cases} u & \text{in } \Omega, \\ 0 & \text{in } \mathbb{R}^d \setminus \Omega. \end{cases} \quad (\text{A.20})$$

As $\text{supp } \bar{u} \subset\subset M$ for every (for example, bounded open Lipschitz) domain $M \supset \Omega$, it follows that $\bar{u} \in H_0^1(M)$. Therefore, in particular, $\bar{u} \in H_0^s(M)$ for all $s \in (1/2, 1)$. With $\mathbb{H}^s(\Omega)$ defined with respect to the Dirichlet Laplacian, as in (10), it is known that, for $s \in (1/2, 1)$, $H_0^s(\Omega) = \mathbb{H}^s(\Omega)$ (see Remark 2.1 in [57] and the paragraph preceding Theorem 2.5 therein). Hence, $\bar{u} \in \mathbb{H}^s(M)$. Suppose that $\lambda > 1$. To simplify the notation, from now on we will refer to $\bar{u}$ simply as u and each time we use the notation u_{λ} (where $u_{\lambda}(x) := u(\lambda x)$), we will mean $\bar{u}_{\lambda}$ (where $\bar{u}_{\lambda}(x) := \bar{u}(\lambda x)$). Clearly, $u_{\lambda} \in H_0^1(\lambda\Omega)$ for all $\lambda > 1$.

Since, by assumption, $u \in H_0^1(\Omega)$, we have that

$$\frac{u_{\lambda} - u}{\lambda - 1} \rightharpoonup x \cdot \nabla u \quad \text{weakly in } L^2(\Omega) \text{ as } \lambda \searrow 1; \quad (\text{A.21})$$

cf. [154, Lemma 4.2] for a proof. Since, again by assumption, $(-\Delta_D)^s u \in L^2(\Omega)$, it follows by passing to the weak limit that

$$\int_{\Omega} (x \cdot \nabla u) (-\Delta_D)^s u \, dx = \left. \frac{d}{d\lambda} \right|_{\lambda \searrow 1} \int_{\Omega} u_{\lambda} (-\Delta_D)^s u \, dx.$$

Next, as a preparation for the application of the scaling property stated in Lemma A.10, we rewrite the expression above in terms of the notation of Lemma A.10 as

$$\int_{\Omega} (x \cdot \nabla u)(-\Delta_D^{\Omega})^s u \, dx = \frac{d}{d\lambda} \Big|_{\lambda \searrow 1} \int_{\Omega} u_{\lambda} (-\Delta_D^{\Omega})^s u \, dx.$$

As $u_{\lambda} \in H_0^1(\lambda\Omega)$ and $u \in H_0^1(\Omega)$, the scaling property of the spectral fractional Laplacian stated in Lemma A.10 implies that

$$\begin{aligned} \int_{\Omega} u_{\lambda}(x)(-\Delta_D^{\Omega})^s u(x) \, dx &= \int_{\Omega} (-\Delta_D^{\Omega})^s u_{\lambda}(x) u(x) \, dx = \lambda^{2s} \int_{\Omega} [(-\Delta_D^{\lambda\Omega})^s u](\lambda x) u(x) \, dx \\ &= \lambda^{2s-d} \int_{\lambda\Omega} [(-\Delta_D^{\lambda\Omega})^s u](x') u(x'/\lambda) \, dx', \end{aligned}$$

where we applied the change of variable $x' = \lambda x$. We then have

$$\begin{aligned} \int_{\Omega} (x \cdot \nabla u)(-\Delta_D)^s u \, dx &= \frac{d}{d\lambda} \Big|_{\lambda \searrow 1} \lambda^{2s-d} \int_{\lambda\Omega} [(-\Delta_D^{\lambda\Omega})^s u](x') u(x'/\lambda) \, dx' \\ &= (2s-d) \int_{\Omega} (-\Delta_D^{\Omega})^s u(x) u(x) \, dx + \frac{d}{d\lambda} \Big|_{\lambda \searrow 1} I_{\lambda} \\ &= (2s-d) \int_{\Omega} u(-\Delta_D^{\Omega})^s u \, dx + \frac{d}{d\lambda} \Big|_{\lambda \searrow 1} I_{\lambda}, \end{aligned} \quad (\text{A.22})$$

with $I_{\lambda} := \int_{\lambda\Omega} [(-\Delta_D^{\lambda\Omega})^s u](x') u(x'/\lambda) \, dx'$. We recall that

$$[(-\Delta_B^{\lambda\Omega})^s u](x') = \sum_{k=1}^{\infty} \frac{\lambda_k^s}{\lambda^{2s}} u_k^{\lambda} \phi'_k(x'), \text{ where } u_k^{\lambda} = \int_{\lambda\Omega} u(x') \phi'_k(x') \, dx', \phi'_k(x') = \frac{1}{\lambda^{d/2}} \phi_k(x'/\lambda)$$

are the scaled eigenfunctions $\{\phi'_k\}_{k \geq 1}$, defined in the proof of Lemma A.10, which are $L^2(\lambda\Omega)$ -orthonormal. Let $\tilde{u}_k := \int_{\lambda\Omega} u(x') \phi_k(x'/\lambda) \, dx'$; hence, we have

$$\tilde{u}_k = \int_{\lambda\Omega} u(x') \phi_k(x'/\lambda) \, dx' = \lambda^{d/2} \int_{\lambda\Omega} u(x') \phi'_k(x') \, dx' = \lambda^{d/2} u_k^{\lambda}. \quad (\text{A.23})$$

By expanding the expression for I_{λ} , it follows that

$$\begin{aligned} I_{\lambda} &= \sum_{k,j=1}^{\infty} \lambda_k^s \lambda^{-2s} \left(\frac{1}{\lambda^{d/2}} \int_{\lambda\Omega} u(x') \phi_k(x'/\lambda) \, dx' \right) u_j \int_{\lambda\Omega} \frac{1}{\lambda^{d/2}} \phi_k(x'/\lambda) \phi_j(x'/\lambda) \, dx' \\ &= \lambda^{-2s} \sum_{k=1}^{\infty} \lambda_k^s u_k \tilde{u}_k = \frac{1}{2} \lambda^{-2s} \sum_{k=1}^{\infty} \lambda_k^s u_k^2 + \frac{1}{2} \lambda^{-2s} \sum_{k=1}^{\infty} \lambda_k^s \tilde{u}_k^2 - \frac{1}{2} \lambda^{-2s} \sum_{k=1}^{\infty} \lambda_k^s (u_k - \tilde{u}_k)^2, \end{aligned} \quad (\text{A.24})$$

where in the last line we have used the equality $ab = \frac{1}{2}a^2 + \frac{1}{2}b^2 - \frac{1}{2}(a-b)^2$.

We have that

$$u_k - \tilde{u}_k = \int_{\Omega} u(x) \phi_k(x) \, dx - \int_{\lambda\Omega} u(x') \phi_k(x'/\lambda) \, dx' = \int_{\Omega} (u(x) - \lambda^d u(\lambda x)) \phi_k(x) \, dx,$$

and therefore (A.24) is equivalent to

$$I_{\lambda} = \frac{1}{2} \lambda^{-2s} \|u\|_{\mathbb{H}^s(\Omega)}^2 + \frac{1}{2} \lambda^{-2s} \sum_{k=1}^{\infty} \lambda_k^s \tilde{u}_k^2 - \frac{1}{2} \lambda^{-2s} \|u - \lambda^d u_{\lambda}\|_{\mathbb{H}^s(\Omega)}^2 = I_{\lambda,1} + I_{\lambda,2}, \quad (\text{A.25})$$

with $I_{\lambda,1} := \frac{1}{2}\lambda^{-2s}\|u\|_{\mathbb{H}^s(\Omega)}^2 + \frac{1}{2}\lambda^{-2s}\sum_{k=1}^{\infty}\lambda_k^s\tilde{u}_k^2$ and $I_{\lambda,2} := -\frac{1}{2}\lambda^{-2s}\|u - \lambda^d u_\lambda\|_{\mathbb{H}^s(\Omega)}^2$.

Next, observe that

$$u(x) - u(\lambda x) = \int_0^1 \frac{d}{d\theta} u(H_\theta(x)) d\theta = (1 - \lambda) \int_0^1 \nabla u(H_\theta(x)) \cdot x d\theta, \quad (\text{A.26})$$

where $H_\theta(x) = \theta x + (1 - \theta)\lambda x$. We shall use this equality to prove that $\|u - u_\lambda\|_{L^2(\Omega)} \rightarrow 0$ as $\lambda \searrow 1$. Note, to this end, that

$$\begin{aligned} \|u - u_\lambda\|_{L^2(\Omega)}^2 &= (1 - \lambda)^2 \int_{\Omega} \left(\int_0^1 \nabla u(H_\theta(x)) \cdot x d\theta \right)^2 dx \\ &\leq (1 - \lambda)^2 \int_{\Omega} \int_0^1 |\nabla u(H_\theta(x)) \cdot x|^2 d\theta dx \\ &= (1 - \lambda)^2 \int_0^1 \int_{M_\theta^\lambda} |\nabla u(x') \cdot x'|^2 (C_\theta^\lambda)^2 C_\theta^\lambda dx' d\theta \\ &= (1 - \lambda)^2 \int_0^1 \|\nabla u \cdot x'\|_{L^2(M_\theta^\lambda)}^2 (C_\theta^\lambda)^3 d\theta, \end{aligned}$$

where in the inequality in the first line we have applied the Cauchy–Schwarz inequality and in the passage from the first to the second line we have used the change of variables $x' := \theta x + (1 - \theta)\lambda x$, $C_\theta^\lambda := 1/(\theta + (1 - \theta)\lambda)$ and $M_\theta^\lambda := (C_\theta^\lambda)^{-1}\Omega$. Since $(C_\theta^\lambda)^{-1} \in [1, \lambda]$ for $\lambda > 1$ sufficiently close to 1 we have $M_\theta^\lambda \subset M$ for a fixed M (contained, for example, in 2Ω) and recalling the natural extension (A.20) of u , it follows that $\|\nabla u \cdot x'\|_{L^2(M_\theta^\lambda)} \leq \|\nabla u \cdot x'\|_{L^2(M)}$. Therefore, because $C_\theta^\lambda \leq 1$, we finally have

$$\|u - u_\lambda\|_{L^2(\Omega)}^2 \leq (1 - \lambda)^2 \|\nabla u \cdot x'\|_{L^2(M)}^2. \quad (\text{A.27})$$

As a consequence, $\|u - u_\lambda\|_{L^2(\Omega)} \rightarrow 0$ as $\lambda \searrow 1$.

Next, we shall prove that for λ close to 1, there exists a constant $C(u)$, dependent on u , but independent of λ , such that $|u - u_\lambda|_{H^1(\Omega)} \leq C(u)$. Then, by (A.27) and using a function space interpolation inequality (analogous to Lemma A.2), we will have for $s \in (1/2, 1)$ that

$$\|u - u_\lambda\|_{\mathbb{H}^s(\Omega)} \leq C \|u - u_\lambda\|_{L^2(\Omega)}^{1-s} \|u - u_\lambda\|_{H^1(\Omega)}^s \leq C(u)(1 - \lambda)^{1-s}, \quad (\text{A.28})$$

which will then imply that $\|u - u_\lambda\|_{\mathbb{H}^s(\Omega)} \rightarrow 0$ as $\lambda \searrow 1$. Assuming that $\lambda < 2$, for example, the existence of such a constant $C(u)$ follows by the application of the Cauchy–Schwarz and triangle inequalities together with the fact that for the natural extension of u we have $|u|_{H^1(M)} < \infty$ for any subset $M \supset \Omega$:

$$\begin{aligned} |u - u_\lambda|_{H^1(\Omega)}^2 &= \int_{\Omega} |\nabla(u(x) - u(\lambda x))|^2 dx = \int_{\Omega} |\nabla u(x) - \lambda(\nabla u)(\lambda x)|^2 dx \\ &= \int_{\Omega} |\nabla u|^2 dx + \lambda^2 \int_{\Omega} |(\nabla u)(\lambda x)|^2 dx - 2\lambda \int_{\Omega} \nabla u(x) \cdot (\nabla u)(\lambda x) dx \\ &\leq |u|_{H^1(\Omega)}^2 + |u|_{H^1(M)}^2 + 2|u|_{H^1(\Omega)}|u|_{H^1(M)} = C(u). \end{aligned}$$

Thus we have shown that $\|u - u_\lambda\|_{\mathbb{H}^s(\Omega)} \rightarrow 0$ as $\lambda \searrow 1$. Hence, by the triangle inequality,

$$\|u - \lambda^d u_\lambda\|_{\mathbb{H}^s(\Omega)} \leq (1 - \lambda^d) \|u\|_{\mathbb{H}^s(\Omega)} + \lambda^d \|u - u_\lambda\|_{\mathbb{H}^s(\Omega)}$$

and therefore we also have $\lim_{\lambda \searrow 1} \|u - \lambda^d u_\lambda\|_{\mathbb{H}^s(\Omega)} = 0$. In addition,

$$\begin{aligned} \frac{d}{d\lambda} \Big|_{\lambda \searrow 1} I_{\lambda,2} &= \frac{d}{d\lambda} \Big|_{\lambda \searrow 1} \left(-\frac{1}{2} \lambda^{-2s} \sum_{k=1}^{\infty} \lambda_k^s \left(\int_{\Omega} (u(x) - \lambda^d u(\lambda x)) \phi_k(x) dx \right)^2 \right) \\ &= s \lim_{\lambda \searrow 1} \|u - \lambda^d u_\lambda\|_{\mathbb{H}^s(\Omega)}^2 - \frac{1}{2} \frac{d}{d\lambda} \Big|_{\lambda \searrow 1} \sum_{k=1}^{\infty} \lambda_k^s \left(\int_{\Omega} (u(x) - \lambda^d u(\lambda x)) \phi_k(x) dx \right)^2 \\ &= -\frac{1}{2} \frac{d}{d\lambda} \Big|_{\lambda \searrow 1} \sum_{k=1}^{\infty} \lambda_k^s \left(\int_{\Omega} (u(x) - \lambda^d u(\lambda x)) \phi_k(x) dx \right)^2 \\ &= -\frac{1}{2} \frac{d}{d\lambda} \Big|_{\lambda \searrow 1} \|u - \lambda^d u_\lambda\|_{\mathbb{H}^s(\Omega)}^2. \end{aligned} \tag{A.29}$$

Because the limit in λ is taken for $\lambda > 1$ decreasing toward 1 and $\lim_{\lambda \searrow 1} \|u - \lambda^d u_\lambda\|_{\mathbb{H}^s(\Omega)} = 0$, we see that the expression appearing on the right-hand side of (A.29) is nonpositive.

We have that

$$\frac{1}{2} \lambda^{-2s} \sum_{k=1}^{\infty} \lambda_k^s \tilde{u}_k^2 = \frac{1}{2} \lambda^d \sum_{k=1}^{\infty} \left(\frac{\lambda_k}{\lambda^2} \right)^s \left(\int_{\lambda\Omega} u(x') \phi'_k(x') dx' \right)^2 = \frac{1}{2} \lambda^d \|u\|_{\mathbb{H}^s(\lambda\Omega)}^2.$$

Hence

$$\frac{d}{d\lambda} \Big|_{\lambda \searrow 1} \frac{1}{2} \lambda^{-2s} \sum_{k=1}^{\infty} \lambda_k^s \tilde{u}_k^2 = \frac{1}{2} d \|u\|_{\mathbb{H}^s(\Omega)}^2 + \frac{1}{2} \frac{d}{d\lambda} \Big|_{\lambda \searrow 1} \|u\|_{\mathbb{H}^s(\lambda\Omega)}^2. \tag{A.30}$$

We notice now that we have a domain monotonicity in the sense that

$$\Omega \subseteq M \implies \|u\|_{\mathbb{H}^s(\Omega)} \geq \|u\|_{\mathbb{H}^s(M)}.$$

In order to see this we can consider the expression for the fractional Laplacian involving the heat semigroup:

$$(-\Delta_D^\Omega)^s u(x) = \frac{1}{\Gamma(-s)} \int_0^\infty (e^{\tau \Delta_D^\Omega} u(x) - u(x)) \frac{1}{\tau^{1+s}} d\tau.$$

We then notice that

$$\|u\|_{\mathbb{H}^s(\Omega)}^2 = \int_{\Omega} (-\Delta_D^\Omega)^s u u dx = \frac{1}{\Gamma(-s)} \int_0^\infty \left(\int_{\Omega} \int_{\Omega} W_\tau^\Omega(x, y) u(x) u(y) dy dx - \int_{\Omega} u(x)^2 dx \right) \frac{1}{\tau^{1+s}} d\tau,$$

$$\begin{aligned} \|u\|_{\mathbb{H}^s(\lambda\Omega)}^2 &= \int_{\lambda\Omega} (-\Delta_D^{\lambda\Omega})^s u u dx = \int_{\Omega} (-\Delta_D^{\lambda\Omega})^s u u dx \\ &= \frac{1}{\Gamma(-s)} \int_0^\infty \left(\int_{\Omega} \int_{\Omega} W_\tau^{\lambda\Omega}(x, y) u(x) u(y) dy dx - \int_{\Omega} u(x)^2 dx \right) \frac{1}{\tau^{1+s}} d\tau. \end{aligned}$$

By the monotonicity of the heat kernels for the Dirichlet Laplacian (cf. [163, 78]) we have, for $\lambda > 1$

$$W_\tau^\Omega(x, y) \leq W_\tau^{\lambda\Omega}(x, y), \quad x, y \in \Omega, \quad \tau > 0.$$

Therefore, as $\Gamma(-s) < 0$ and u is assumed to be nonnegative, this immediately implies

$$\|u\|_{\mathbb{H}^s(\Omega)} \geq \|u\|_{\mathbb{H}^s(\lambda\Omega)}.$$

This fact implies that the last term on the right-hand side of (A.30) is nonpositive.

In this way, we have from (A.25) that

$$\begin{aligned} \frac{d}{d\lambda} \Big|_{\lambda \searrow 1} I_\lambda &= \frac{d}{d\lambda} \Big|_{\lambda \searrow 1} I_{\lambda,1} + \frac{d}{d\lambda} \Big|_{\lambda \searrow 1} I_{\lambda,2} \\ &\leq \frac{d}{d\lambda} \Big|_{\lambda \searrow 1} I_{\lambda,1} = -s \|u\|_{\mathbb{H}^s(\Omega)}^2 + \frac{d}{2} \|u\|_{\mathbb{H}^s(\Omega)}^2 = \frac{1}{2}(-2s + d) \|u\|_{\mathbb{H}^s(\Omega)}^2 \end{aligned}$$

Returning to (A.22) we then arrive at the desired final result. □

Remark A.12. The monotonicity relationship

$$\Omega \subseteq M \implies \|u\|_{\mathbb{H}^s(\Omega)} \geq \|u\|_{\mathbb{H}^s(M)},$$

that was used in the proof of Lemma A.11 might seem counterintuitive. However, we present a one-dimensional example that shows that this fact is true for functions defined in Ω and extended by zero outside of it.

Let us consider $\Omega = (-1, 1)$, $\lambda = 2$, $s = 1/2$ and $u(x) = \cos(\pi x/2)$. The eigenfunctions and corresponding eigenvalues of the Dirichlet Laplacian on Ω are given by

$$\phi_k(x) = \begin{cases} \cos\left(\frac{k\pi x}{2}\right) & \text{if } k \text{ odd,} \\ \sin\left(\frac{k\pi x}{2}\right) & \text{if } k \text{ even,} \end{cases} \quad \lambda_k = \left(\frac{k\pi}{2}\right)^2,$$

while those on $\lambda\Omega$ are

$$\phi'_k(x) = \frac{1}{\sqrt{\lambda}} \phi_k\left(\frac{x}{\lambda}\right), \quad \lambda_k = \left(\frac{k\pi}{2\lambda}\right)^2.$$

By the fact that $\cos(\pi x/2) = \phi_1(x)$, we clearly have

$$\int_{-1}^1 \cos\left(\frac{\pi x}{2}\right) \cos\left(\frac{k\pi x}{2}\right) dx = \begin{cases} 1 & \text{if } k = 1, \\ 0 & \text{otherwise.} \end{cases}$$

Since $\cos(\pi x/2)$ is an even function, to compute $\|\cdot\|_{\mathbb{H}^s(\lambda\Omega)}$, we need only to compute the modes corresponding to $\cos$ functions, that is for k odd, and thus

$$\int_{-1}^1 \cos\left(\frac{\pi x}{2}\right) \frac{1}{\sqrt{\lambda}} \cos\left(\frac{k\pi x}{2\lambda}\right) dx = \frac{4\lambda^{3/2} \cos(\frac{k\pi}{2\lambda})}{\pi(\lambda^2 - k^2)}.$$

Thus, for $\lambda = 2$ and $s = 1/2$, we have

$$\|u\|_{\mathbb{H}^s(\Omega)}^2 = \left(\frac{\pi}{2}\right)^{2s} = \frac{\pi}{2}$$

and

$$\begin{aligned} \|u\|_{\mathbb{H}^s(\lambda\Omega)}^2 &= \sum_{\substack{k=1 \\ k \text{ odd}}}^{\infty} \left(\frac{k\pi}{2\lambda}\right)^{2s} \frac{16\lambda^3 \cos^2(\frac{k\pi}{2\lambda})}{\pi^2(\lambda^2 - k^2)^2} = \sum_{\substack{k=1 \\ k \text{ odd}}}^{\infty} \frac{k\pi}{4} \frac{16 \cdot 8 \cos^2(\frac{k\pi}{4})}{\pi^2(4 - k^2)^2} = \sum_{\substack{k=1 \\ k \text{ odd}}}^{\infty} \frac{k}{4} \frac{16 \cdot 4}{\pi(4 - k^2)^2} \\ &= \frac{16}{\pi} \sum_{\substack{k=1 \\ k \text{ odd}}}^{\infty} \frac{k}{(4 - k^2)^2} = \frac{16}{\pi} \sum_{m=0}^{\infty} \frac{2m+1}{(4 - (2m+1)^2)^2} \\ &= \frac{16}{\pi} \sum_{m=0}^{\infty} \frac{1}{8} \left(\frac{1}{(2m-1)^2} - \frac{1}{(2m+3)^2} \right) \\ &= \frac{2}{\pi} \cdot 2 = \frac{4}{\pi} < \frac{\pi}{2} = \|u\|_{\mathbb{H}^s(\Omega)}^2, \end{aligned}$$

where in the passage from the third to the fourth line we used the fact that the series, as written in the third line, is a telescoping series.

Lemma A.13. *Assume the same hypotheses as in Lemma A.10 and consider the problems*

$$(-\Delta_{\mathcal{B}}^{\Omega})^s u = f, \quad f \in H^1(\Omega), \quad \text{and} \quad (-\Delta_{\mathcal{B}}^{\lambda\Omega})^s \bar{u} = \bar{f}, \quad \bar{f} \in H^1(\lambda\Omega), \quad (\text{A.31})$$

where $\bar{f}$ is an extension or restriction f on $\lambda\Omega$ respectively if $\lambda > 1$ or $\lambda < 1$, such that $\bar{f} = f$ on Ω . Then, $\bar{u} \rightarrow u$ in $\mathbb{H}^s(\Omega)$ as $\lambda \rightarrow 1$.

Proof. Similarly as in Lemma A.10, we shall use the notation $f_{\lambda}(x) = \bar{f}(\lambda x)$. By the same argument as in Lemma A.10 we have $((-\Delta_{\mathcal{B}}^{\lambda\Omega})^{-s} \bar{f})(x) = \lambda^{2s} (-\Delta_{\mathcal{B}}^{\Omega})^{-s} (f_{\lambda}(x/\lambda))$. Hence,

$$\bar{u}(x) - u(x) = ((-\Delta_{\mathcal{B}}^{\lambda\Omega})^{-s} \bar{f})(x) - (-\Delta_{\mathcal{B}}^{\Omega})^{-s} f(x) = (-\Delta_{\mathcal{B}}^{\Omega})^{-s} (\lambda^{2s} \bar{f}(x) - f(x)).$$

Therefore,

$$\begin{aligned} \|\bar{u} - u\|_{\mathbb{H}^s(\Omega)}^2 &= ((-\Delta_{\mathcal{B}}^{\Omega})^s (\bar{u} - u), \bar{u} - u) = (\lambda^{2s} \bar{f} - f, (-\Delta_{\mathcal{B}}^{\Omega})^{-s} (\lambda^{2s} \bar{f} - f)) \\ &\leq \|\lambda^{2s} \bar{f} - f\|_{L^2(\Omega)} \|(-\Delta_{\mathcal{B}}^{\Omega})^{-s} (\lambda^{2s} \bar{f} - f)\|_{L^2(\Omega)} \\ &\leq C \|\lambda^{2s} \bar{f} - f\|_{L^2(\Omega)}^2, \end{aligned}$$

where in the passage from the first to the second line we have used the Cauchy–Schwarz inequality, and in the passage from the second to the third line we have used the bound on the solution of a fractional Poisson equation with spectral fractional Laplacian in terms of the source term (A.3). Using the proof of [154, Lemma 4.2], we have that $\|\lambda^{2s} \bar{f} - f\|_{L^2(\Omega)}^2$ tends to zero as $\lambda \rightarrow 1$. This completes the proof. $\square$

B

The integral fractional Laplacian

We report auxiliary results for the integral definition of the fractional Laplacian (4) and the related space $H^s(\mathbb{R}^d)$ (6).

For Ω an open and bounded subset of $\mathbb{R}^d$, let δ be the regularised distance to the boundary function, that we defined in (4.8). We first make the observation that for $C^{1,1}$ domains the power s of the regularized distance function δ belongs to V . We recall that $d_\Omega(x) = \text{dist}(x, \mathbb{R}^d \setminus \Omega)$ for $x \in \mathbb{R}^d$.

Lemma B.1. *Assume that $\partial\Omega \in C^{1,1}$ and that $\delta \in W^{1,\infty}(\Omega)$ satisfies $c\delta \leq d_\Omega \leq C\delta$, for some positive constants c, C . Then, $\delta^s \in H^s(\mathbb{R}^d)$ for all $s \in (0, 1)$.*

Proof. Let us decompose the integral taking advantage of the symmetry in x and y

$$\begin{aligned} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{|\delta(x)^s - \delta(y)^s|^2}{|x - y|^{d+2s}} dy dx &= \int_{\Omega} \int_{\Omega} \frac{|\delta(x)^s - \delta(y)^s|^2}{|x - y|^{d+2s}} dy dx \\ &\quad + 2 \int_{\Omega} \int_{\mathbb{R}^d \setminus \Omega} \frac{|\delta(x)^s - \delta(y)^s|^2}{|x - y|^{d+2s}} dy dx \end{aligned}$$

If $x \in \Omega$ then we use that $\mathbb{R}^d \setminus \Omega \subset \mathbb{R}^d \setminus B(x, d_\Omega(x))$ to estimate

$$\int_{\mathbb{R}^d \setminus \Omega} \frac{|\delta(x)^s - \delta(y)^s|^2}{|x - y|^{d+2s}} dy \leq C\delta(x)^{2s} \int_{d_\Omega(x)}^{\infty} r^{-d-2s} r^{d-1} dr = C\delta(x)^{2s} d_\Omega(x)^{-2s},$$

where in the first inequality we have used the change of variables in radial coordinates $|x - y| = r$; here and henceforth C signifies a generic positive constant. Therefore, we can integrate in x to obtain that the integral in $\Omega \times (\mathbb{R}^d \setminus \Omega)$ is finite. In order to deal with the integral in $\Omega \times \Omega$ we point out that

$$|\delta(x)^s - \delta(y)^s| \leq \int_0^1 \left| \frac{d}{d\theta} \delta(\theta x + (1 - \theta)y) \right|^s d\theta \leq C \min\{\delta(x), \delta(y)\}^{s-1} |x - y|.$$

Using Lipschitz regularity, we also have the following estimate

$$|\delta(x)^s - \delta(y)^s| \leq C|\delta(x) - \delta(y)|^s \leq C|x - y|^s.$$

Therefore, we have that

$$\begin{aligned} \int_{\Omega} \int_{\Omega} \frac{|\delta(x)^s - \delta(y)^s|^2}{|x - y|^{d+2s}} dy dx &\leq C \int_{\Omega} \int_{\Omega} \min\{\delta(x), \delta(y)\}^{s-1} |x - y|^{-d-s+1} dy dx \\ &\leq C \int_{\Omega} \int_{\Omega} \min\{d_{\Omega}(x), d_{\Omega}(y)\}^{s-1} |x - y|^{-d-s+1} dy dx \\ &= 2C \int_{\Omega} d_{\Omega}(x)^{s-1} \int_{\{y \in \Omega: d_{\Omega}(x) < d_{\Omega}(y)\}} |x - y|^{-d-s+1} dy dx. \end{aligned}$$

On the one hand, we can estimate

$$\int_{\{y \in \Omega: d_{\Omega}(x) < d_{\Omega}(y)\}} |x - y|^{-d-s+1} dy \leq \int_{B(x, \text{diam}(\Omega))} |x - y|^{-d-s+1} dy = C \text{diam}(\Omega)^{1-s}.$$

Since $\Omega \in C^{1,1}$ we can use the tubular neighbourhood theorem to prove that

$$\int_{\Omega} d_{\Omega}(x)^{s-1} dx < \infty. \quad \square$$

Lemma B.2. *Let $s \in (0, 1)$ and $\alpha \in (s, 1]$. Let $v \in W^{\alpha, \infty}(\mathbb{R}^d)$ such that $\text{supp } v \subset B_R$ for some R . Then $v \in H^s(\mathbb{R}^d)$ and*

$$|v|_{H^s(\mathbb{R}^d)} \leq C_{d,s,R} \left(\|v\|_{L^{\infty}(\mathbb{R}^d)} + \frac{1}{\sqrt{\alpha - s}} |v|_{W^{\alpha, \infty}(\mathbb{R}^d)} \right).$$

Proof. We will use the same name for different constants, just keep tracking of their dependence.

Let us denote $g(x, y) = \frac{|v(x) - v(y)|^2}{|x - y|^{d+2s}}$. Then,

$$\begin{aligned} |v|_{H^s(\mathbb{R}^d)}^2 &= \iint_{B_R \times B_R} g(x, y) dx dy + 2 \iint_{\substack{B_R \times (\mathbb{R}^d \setminus B_R) \\ |x - y| \leq 1}} g(x, y) dx dy + 2 \iint_{\substack{B_R \times (\mathbb{R}^d \setminus B_R) \\ |x - y| > 1}} g(x, y) dx dy \\ &:= I_1 + I_2 + I_3. \end{aligned}$$

We now estimate each term in the above equality. First,

$$\begin{aligned} I_1 &= |v|_{W^{\alpha, \infty}(\mathbb{R}^d)}^2 \iint_{B_R \times B_R} \frac{|x - y|^{2\alpha}}{|x - y|^{d+2s}} dx dy \leq C_{d,R} |v|_{W^{\alpha, \infty}(\mathbb{R}^d)}^2 \int_0^{2R} r^{2\alpha-1-2s} dr \\ &\leq \frac{C_{d,R}}{\alpha - s} |v|_{W^{\alpha, \infty}(\mathbb{R}^d)}^2, \end{aligned}$$

where $C_{d,R}$ stands for a positive constant depending only on d and R . Similarly, we have that

$$I_2 \leq 2 \iint_{B_{R+1} \times B_{R+1}} g(x, y) dx dy \leq \frac{C_{d,R}}{\alpha - s} |v|_{W^{\alpha, \infty}(\mathbb{R}^d)}^2.$$

Finally, we deduce

$$I_3 \leq 4 \|v\|_{L^{\infty}(\mathbb{R}^d)}^2 \int_{B_R} \int_{|x - y| > 1} \frac{1}{|x - y|^{d+2s}} dx dy = C_{d,s,R} \|v\|_{L^{\infty}(\mathbb{R}^d)}^2,$$

where $C_{d,R}$ stands for a positive constant depending only on d , s and R . The proof is completed by observing that $(a^2 + b^2)^{\frac{1}{2}} \leq |a| + |b|$ for all $a, b \in \mathbb{R}$. $\square$

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