A SPECTRALLY ACCURATE APPROXIMATION TO SUBDIFFUSION EQUATIONS USING THE LOG ORTHOGONAL FUNCTIONS*

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Abstract. In this paper, we develop and analyze a spectral-Galerkin method for solving subdiffusion equations, which contain Caputo fractional derivatives with order $\nu \in (0, 1)$. The basis functions of our spectral method are constructed by applying a log mapping to Laguerre functions and have already been proved to be suitable to approximate functions with fractional power singularities in [S. Chen and J. Shen, *Log Orthogonal Functions: Approximation Properties and Applications*, preprint, arXiv:2003.01209[math.NA], 2020]. We provide rigorous regularity and error analysis which show that the scheme is spectrally accurate, i.e., the convergence rate depends only on regularity of problem data. The proof relies on the approximation properties of some reconstruction of the basis functions as well as the sharp regularity estimate in some weighted Sobolev spaces. Numerical experiments fully support the theoretical results and show the efficiency of the proposed spectral-Galerkin method. We also develop a fully discrete scheme with the proposed spectral method in time and the Galerkin finite element method in space, and apply the proposed techniques to subdiffusion equations with time-dependent diffusion coefficients as well as to the nonlinear time-fractional Allen–Cahn equation.

Key words. log orthogonal functions, subdiffusion equation, singularity, error analysis, spectral accuracy

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1. Introduction. Let $\Omega \subset \mathbb{R}^d$ $(d = 1, 2, 3)$ be a bounded domain with a convex polygonal boundary $\partial\Omega$. Consider the following time-fractional evolution problem for the function $u(x, t)$ with $\nu \in (0, 1)$:

$$
(1.1) \quad
\begin{cases}
{}^{C}_{0}\mathrm{D}^{\nu}_{t} u(x, t) = Lu(x, t) + f(x, t), & x \in \Omega, \ t \in \Lambda := (0, T), \\
u(x, t) = 0, & (x, t) \in \partial\Omega \times (0, T], \\
u(x, 0) = u_0(x), & x \in \Omega,
\end{cases}
$$

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where $T > 0$ is a fixed final time, f and u_0 are given source term and initial data, respectively, and ${}^{C}_{0}\mathrm{D}^{\nu}_{t}$ denotes the Caputo fractional derivative with respect to t and defined by [33, p. 70]

$$ {}^{C}_{0}\mathrm{D}^{\nu}_{t} y(t) = \frac{1}{\Gamma(1-\nu)} \int_0^t (t-\tau)^{-\nu} y'(\tau) \mathrm{d}\tau; $$

here $Lu = \nabla \cdot (a(x)\nabla u) - b(x)u$ and $a(x)$ is a symmetric $d \times d$ matrix-valued measurable function on the domain Ω with smooth entries, and $b(x) \geq 0$ is an $L_\infty(\Omega)$-function. We assume that

$$ (1.2) \qquad c_0|\xi|^2 \leq \xi^T a(x)\xi \leq c_1|\xi|^2 \qquad \text{for any} \quad \xi \in \mathbb{R}^d,\ x \in \Omega, $$

where $c_0, c_1 > 0$ are constants. Then $-L$ is a symmetric and positive definite operator.

In recent years, the model (1.1) has received a growing interest in mathematical analysis and numerical simulation, due to its capability to describe anomalous diffusion processes, in which the mean square variance of particle displacements grows sublinearly with the time, instead of the linear growth for a Gaussian process. Nowadays, the model has been successfully employed in many practical applications, e.g., diffusion in media with fractal geometry [48], ion transport in column experiments [18], and non-Fickian transport in geological formation [6], to name but a few; see [45] for an extensive list.

The literature on the numerical analysis of the subdiffusion problem is vast; see [24, 31, 30, 62] for a rather incomplete list of the spatially semidiscrete scheme. In contrast with the classical parabolic counterpart, the fractional differential operator appearing in the diffusion model often leads to limited regularity of the solution, which results in low accuracy of many popular time-stepping methods [56]. It has been proved that the piecewise linear polynomial collocation method with uniform meshes [37, 58] is only first-order accurate, due to the presence of the initial layer caused by the fractional differential operator. Similarly, the convolution quadrature [39, 12] generated by backward differential formulas (BDFs) for solving the model (1.1) has only first-order accuracy [27], while the high-order convergence rates could be restored by correcting the first several time steps. See also [57, 36, 34] for studies on the $L1$ scheme with graded meshes, [63] for the analysis of the $L1$ scheme with initial correction, [16, 5] for the convolution quadrature Runge–Kutta schemes, [43, 47, 44] for the application of the discontinuous Galerkin method, and [3, 4, 22, 38, 60] for some fast algorithms.

Compared with time-stepping schemes, spectral methods with specially constructed basis functions (see [7, 9, 41, 8, 66, 21, 53, 68, 69]) could compensate for the weakly singular behavior of functions and hence are expected to approximate the solution of (1.1) accurately. Indeed, some efficient spectral/spectral collocation methods based on the generalized Jacobi functions (or polyfractonomials) are proposed in [65, 66] for some fractional models. In [10], Chen, Shen, and Wang studied approximation properties of generalized Jacobi polynomials in weighted Sobolev spaces and used them to develop a spectral Petrov–Galerkin method for fractional ODEs without low-order terms. Exponential convergence was theoretically confirmed, provided reasonable assumptions on the smoothness of problem data. However, the analysis relies on the fact that suitable fractional derivatives of the solution are smooth despite the solution itself being nonsmooth, so it cannot be straightforwardly extended to the subdiffusion equation (1.1). According to the singularity of the underlying fractional problems, the Müntz spectral method based on a nonlinear mapping to Jacobi polynomials was

proposed in [20, 21] to enhance the algebraic convergence rate. Our study is motivated by a very recent work of Chen and Shen [9], where a spectral method was developed by using novel log orthogonal functions (LOFs), which were constructed by applying a log mapping to the Laguerre functions and can approximate weakly singular solutions of fractional ODEs with spectral accuracy. This merit leads us to use LOFs to handle the singularity that has arisen in the time direction of the time-fractional evolution problem.

The main contribution of this paper is to develop a spectral-Galerkin method in time with LOFs for solving the subdiffusion problem (1.1) and to show the spectral accuracy, provided some reasonable assumptions on the smoothness of problem data. In particular, we prove that if $u_0 \in \dot{H}^3(\Omega)$ and for any fixed integer m

(1.3)
$$\int_0^T t^{2j} \|f^{(j)}(t)\|_{H_0^1(\Omega)}^2 |\log(t/T)|^k \, \mathrm{d}t < \infty \quad \text{for all} \ \ 0 \le j \le k \ \ \text{and} \ \ k = 0, 1, \ldots, m,$$

then $_0\mathrm{D}_t^{\frac{\nu}{2}} u(x,t)$ belongs to the nonuniformly weighted Sobolev space $A_{\frac{\beta}{2},T}^m(\Lambda; H_0^1(\Omega))$ with some mapping parameter $\beta > 0$ (defined in section 3.4), and there holds the error estimate (Theorem 4.5)

$$\|u_N - u\|_{H^{\frac{\nu}{2}}(\Lambda; L^2(\Omega))}^2 + \|\nabla(u_N - u)\|_{L^2(\Lambda; L^2(\Omega))}^2 \le cN^{-m},$$

where u_N is the solution of the Galerkin spectral method using N basis functions (LOFs), and the generic constant c is independent of N and u but may depend on ν, β, m, T, u_0, and f. We believe that this is the first such result with spectral accuracy in time for weakly singular solutions of subdiffusion problem (1.1). Moreover, we also study the fully discrete scheme with the proposed spectral method in time and Galerkin finite element method in space, and develop a fast algorithm to solve the matrix system.

It should be noted that the proposed approach is not limited to the linear subdiffusion problem with time-independent diffusion coefficients (1.1). Compared with the high-order BDF schemes [27] and the Runge–Kutta schemes [16, 5], which require that the source term is sufficiently smooth in the time direction, the current numerical scheme allows singularity of the source term near $t = 0$ and hence performs well even for solving linear subdiffusion equations with time-dependent diffusion coefficients as well as nonlinear subdiffusion problems (see, e.g., section 5, Examples (b) and (c)). We present numerical results to support our theoretical findings and to show the significant advantages of the proposed method.

The rest of the paper is organized as follows. In section 2, we will provide some background on fractional calculus and introduce the solution representation to (1.1) by spectral decomposition. In section 3, we will introduce the LOFs and their approximation properties. A spectral-Galerkin method using log orthogonal basis functions will be developed in section 4, and the error analysis will be provided. A fully discrete scheme and a fast algorithm to solve the matrix system will also be discussed. In section 5, we will provide some numerical experiments to show the efficiency and accuracy of the proposed spectral-Gakerkin method for solving the linear subdiffusion equation (1.1) and apply the proposed techniques to solve subdiffusion equations with time-dependent diffusion coefficients (5.6) and nonlinear subdiffusion models (5.14).

2. Preliminaries.

2.1. Fractional integrals and derivatives. To begin with, we shall review the definitions of the fractional integrals and fractional derivatives and some important

basic properties. We recommend that potential readers refer to [49, 51], [35, Lemma 2.6 and Lemma 2.8], and [15, Corollary 2.15] for the details of the following results.

DEFINITION 2.1 (fractional integrals and derivatives). *For $t \in \Lambda = (0,T)$ and $\rho \in \mathbb{R}^+$, the left and right fractional integrals are respectively defined as*

$$_0\mathrm{I}_t^\rho f(t) = \frac{1}{\Gamma(\rho)} \int_0^t \frac{f(\tau)}{(t-\tau)^{1-\rho}} dy, \quad _t\mathrm{I}_T^\rho f(t) = \frac{1}{\Gamma(\rho)} \int_t^T \frac{f(\tau)}{(\tau-t)^{1-\rho}} d\tau.$$

For real $s \in [k-1, k)$ with $k \in \mathbb{N}$, the Riemann–Liouville fractional derivatives are defined by

$$_0\mathrm{D}_t^s f(t) = \partial_t^k \{_0\mathrm{I}_t^{k-s} f(t)\}, \quad _t\mathrm{D}_T^s f(t) = (-1)^k \partial_t^k \{_t\mathrm{I}_T^{k-s} f(t)\}.$$

The Caputo fractional derivative of order s is defined by

$$_0^C\mathrm{D}_t^s f(x) = {_0\mathrm{I}_t^{k-s}} \{\partial_t^k f(t)\}, \quad _t^C\mathrm{D}_1^s f(t) = (-1)^k {_t\mathrm{I}_T^{k-s}} \{\partial_t^k f(t)\}.$$

The derivative operator $\partial_t^k := \frac{d^k}{dt^k}$, for notational simplicity, will be used throughout this paper.

If $f(0) = 0$, then it holds that

$$(2.1) \qquad _0^C\mathrm{D}_t^\nu f(t) = {_0\mathrm{D}_t^\nu} f(t), \quad 0 < \nu < 1.$$

To establish a variational formula for (1.1), we introduce some fractional Hilbert spaces. For any $\beta \geq 0$, we denote $H^\beta(\Lambda)$ to be the Sobolev space of order β on the interval Λ (see [1]), and $H_0^\beta(\Lambda)$ the set of functions f in $H^\beta(\Lambda)$ whose extension by zero to $\mathbb{R}$ is in $H^\beta(\mathbb{R})$, with the seminorm $|f|_{H_0^\beta(\Lambda)} = |\widetilde{f}|_{H^\beta(\mathbb{R})}$. For $0 \leq \beta < 1/2$, it is well known that $H_0^\beta(\Lambda)$ coincides with $H^\beta(\Lambda)$.

In [23, Theorems 2.1 and 3.1], it has been proved that for any $f \in H_0^\beta(\Lambda)$ with $\beta \in (0,1)$, there exist $c_{\beta,1}$ and $c_{\beta,2}$ such that

$$(2.2) \qquad c_{\beta,1} \|_0\mathrm{D}_t^\beta f\|_{L^2(\Lambda)} \leq |f|_{H_0^\beta(\Lambda)} \leq c_{\beta,2} \|_0\mathrm{D}_t^\beta f\|_{L^2(\Lambda)}.$$

Moreover, for any $f, g \in H_0^\beta(\Lambda)$ with $0 \leq \beta < 1/2$, it has been proved in [35, Lemma 2.8] that

$$(2.3) \qquad (_0\mathrm{D}_t^{2\beta} f, g)_\Lambda = (_0\mathrm{D}_t^\beta f, {_t\mathrm{D}_T^\beta} g)_\Lambda,$$

where $(\cdot, \cdot)_\Lambda$ denotes the inner product of $L^2(\Lambda)$ or the duality between $H_0^s(\Lambda)$ and its dual space $(H_0^s(\Lambda))^* = H^{-s}(\Lambda)$ with $s \in [0,1]$. Note that the fractional operator $_0\mathrm{D}_t^\beta f$ is defined in the distribution sense as in [35], or $_0\mathrm{D}_t^{2\beta} f$ is not well defined for $f \in H_0^\beta(\Lambda)$. In addition, given $f \in H_0^\beta(\Lambda)$, the following coercivity is valid:

$$(2.4) \qquad (_0\mathrm{D}_t^\beta f, {_t\mathrm{D}_T^\beta} f)_\Lambda \geq c_\beta |f|_{H_0^\beta(\Lambda)}^2.$$

We shall use extensively Bochner–Sobolev spaces $H_0^\beta(\Lambda; L^2(\Omega))$. For any $\beta \in (0,1)$, we denote by $H_0^\beta(\Lambda; L^2(\Omega))$ the space of functions u with the norm defined as

$$|u|_{H_0^\beta(\Lambda; L^2(\Omega))}^2 = \int_\mathbb{R} \int_\mathbb{R} \frac{\|\widetilde{u}(t) - \widetilde{u}(s)\|_{L^2(\Omega)}^2}{|t-s|^{1+2\beta}} \, ds \, dt.$$

Besides, we recall the important equivalence inequality that for $\beta \in (0, 1/2)$

$$(2.5) \qquad c_{\beta,1} \|_0\mathrm{D}_t^\beta u\|_{L^2(\Lambda; L^2(\Omega))}^2 \leq |u|_{H_0^\beta(\Lambda; L^2(\Omega))}^2 \leq c_{\beta,2} \|_0\mathrm{D}_t^\beta u\|_{L^2(\Lambda; L^2(\Omega))}^2.$$

2.2. Reformulation of original problem. In our paper, we shall study an equivalent reformulation of the original subdiffusion problem (1.1). In case that $u_0 \in H^2(\Omega) \cap H_0^1(\Omega)$, we let $w = u - u_0$ and observe that w satisfies

$$\begin{cases} {}_0^C\mathrm{D}_t^\nu w(x,t) = Lw(x,t) + F(x,t), & x \in \Omega, \ t \in \Lambda := (0,T), \\ w(x,t) = 0, & (x,t) \in \partial\Omega \times (0,T], \\ w(x,0) = 0, & x \in \Omega, \end{cases}$$

with $F(x,t) = f(x,t) + Lu_0$. Since $w(0) = 0$, we have ${}_0^C\mathrm{D}_t^\nu w(t) = {}_0\mathrm{D}_t^\nu w(t)$ by (2.1). Then, without loss of generality, we only consider the following subdiffusion problem with trivial initial data:

$$(2.6) \qquad \begin{cases} {}_0\mathrm{D}_t^\nu u(x,t) = Lu(x,t) + f(x,t), & x \in \Omega, \ t \in \Lambda := (0,T), \\ u(x,t) = 0, & (x,t) \in \partial\Omega \times (0,T], \\ u(x,0) = 0, & x \in \Omega. \end{cases}$$

The case of a nonsmooth initial condition, e.g., $u_0 \in L^2(\Omega)$, requires new techniques and is out of the scope of the current paper.

2.3. Solutions to subdiffusion equations. In this section, we introduce a representation of the solution to (1.1) by spectral decomposition, which will be intensively used in the error analysis. To this end, we consider the eigenvalue problem

$$-L\varphi = \lambda\varphi \text{ in } \Omega \qquad \text{and} \qquad \varphi_n = 0 \text{ on } \partial\Omega.$$

Since $-L$ is a symmetric uniformly elliptic operator, it admits a nondecreasing sequence $\{\lambda_j\}_{j=1}^\infty$ of positive eigenvalues, which tend to ∞ with $j \to \infty$, and a corresponding sequence $\{\varphi_j\}_{j=1}^\infty$ of eigenfunctions, $\varphi_j \in \mathrm{Dom}(L) = H_0^1(\Omega) \cap H^2(\Omega)$, forms an orthonormal basis in $L^2(\Omega)$, whose inner product is denoted by $(\cdot,\cdot)_\Omega$. Further, $\|v\|_{\dot{H}^0(\Omega)} = \|v\|_{L^2(\Omega)} = (v,v)_\Omega^{1/2}$ is the norm in $L^2(\Omega)$. Besides, it is easy to verify that $\|v\|_{\dot{H}^1(\Omega)} = \|\nabla v\|_{L^2(\Omega)}$ is also the norm in $H_0^1(\Omega)$ and $\|v\|_{\dot{H}^2(\Omega)} = \|\Delta v\|_{L^2(\Omega)}$ is equivalent to the norm in $H^2(\Omega) \cap H_0^1(\Omega)$ (cf. [59, Lemma 3.1]).

Next, we represent the solution to problem (2.6) using the eigenpairs $\{(\lambda_j, \varphi_j)\}_{j=1}^\infty$. Define an operator $E(t)$ for $v \in L^2(\Omega)$ by

$$E(t)v(x) = \sum_{j=1}^\infty t^{\nu-1} E_{\nu,\nu}(-\lambda_j t^\nu)\,(v,\varphi_j)_\Omega\,\varphi_j(x),$$

where $E_{a,b}(z)$ denotes the two-parameter Mittag–Leffler function:

$$E_{a,b}(z) = \sum_{j=0}^\infty \frac{z^j}{\Gamma(aj+b)}, \quad z \in \mathbb{C}, \ a > 0, \ b \in \mathbb{R}.$$

The Mittag–Leffler function plays a crucial role in solving fractional differential equations. A lot of useful properties can be found in [19, 33, 49]. For clarity, here we list some results which will be used in the subsequent sections below.

LEMMA 2.2. *Let* $0 < a < 2$, $b \in \mathbb{R}$, *and* $a\pi/2 < \mu < \min(\pi, a\pi)$. *There exists a constant* $C = C(a,b,\mu) > 0$ *such that*

$$|E_{a,b}(z)| \leq \frac{C}{1+|z|}, \quad \mu \leq |\arg(z)| \leq \pi.$$

LEMMA 2.3. *For $\lambda > 0$, $a > 0$, and $b \in \mathbb{R}$ and fixed positive integer k, we have*

$$(2.7) \qquad \partial_t^k \{t^{b-1} E_{a,b}(-\lambda t^a)\} = t^{b-k-1} E_{a,b-k}(-\lambda t^a), \quad t > 0.$$

In particular, for $b = 1$ and $b = a$, there exists

$$\partial_t^k E_{a,1}(-\lambda t^a) = -\lambda t^{a-k} E_{a,a-k+1}(-\lambda t^a),$$
$$\partial_t^k \{t^{a-1} E_{a,a}(-\lambda t^a)\} = t^{a-k-1} E_{a,a-k}(-\lambda t^a),$$

where $\partial_t^k := \frac{\mathrm{d}^k}{\mathrm{d}t^k}$ is the k-fold derivative with respect to t.

Proof. The proof can be ended by the following relation:

$$\partial_t^k \{t^{b-1} E_{a,b}(-\lambda t^a)\} = \partial_t^k \sum_{j=0}^{\infty} \frac{(-\lambda)^j t^{ja+b-1}}{\Gamma(ja+b)} = t^{b-k-1} E_{a,b-k}(-\lambda t^a)$$

for any $t > 0$.   □

Then the solution to (2.6) could be expressed as (see [50, Theorem 2.1])
$$(2.8)$$
$$u(x,t) = \int_0^t E(t-s)f(s)\, ds := \sum_{n=1}^{\infty} \int_0^t \tau^{\nu-1} E_{\nu,\nu}(-\lambda_n \tau^\nu)\big(f(\cdot, t-\tau), \varphi_n\big)_\Omega \varphi_n(x)\mathrm{d}\tau.$$

Remark 2.1. From the series expansion of the Mittag–Leffler function, it is easy to observe that the solution (2.8) is weakly singular near $t = 0$. This leads to low accuracy of many popular time-stepping methods. For example, in the case where $f(x,t) \equiv f(x)$, the solution can be written as

$$u(x,t) = \sum_{n=1}^{\infty} \int_0^t \tau^{\nu-1} E_{\nu,\nu}(-\lambda_n \tau^\nu)\mathrm{d}\tau \; \big(f, \varphi_n\big)_\Omega \; \varphi_n(x)$$
$$= \sum_{n=1}^{\infty} \frac{1}{\lambda_n} E_{\nu,1}(-\lambda_n \tau^\nu)\big(f, \varphi_n\big)_\Omega \; \varphi_n(x).$$

In fact, Lemma 2.3 indicates that, for $m \geq 1$, the m-fold derivative $\partial_t^m E_{\nu,1}(-\lambda t^\nu) \notin L^1(0,T)$. As a result, the solution of the subdiffusion model fails to meet the regularity assumptions of many existing algorithms. In order to get rid of this dilemma, we introduce the following log orthogonal functions, which can approximate the Mittag–Leffler functions with an exponential convergence rate.

3. Log orthogonal functions (LOFs). In order to design an efficient spectral method in the time direction of the subdiffusion equation, we shall use the following LOFs:
$$\mathcal{S}_n(t) := \mathcal{S}_n(t;\beta) = t^{\beta/2} \mathcal{L}_n(-(\beta+1)\log t), \quad t \in (0,1),$$

where $\mathcal{L}_n(x) = \mathcal{L}_n(-(\beta+1)\log t)$ is the classical Laguerre polynomial of the variable $x \in (0,\infty)$. The mapping parameter β is designed for handling functions with distinct singular behavior when t is close to 0 (see [9]).

The LOFs were proposed by Chen and Shen [9] very recently for solving ODEs with one point singularity. We will see in subsequent sections that the new method based on LOFs perfectly circumvents the obstacle caused by the singularity of the solution of the subdiffusion equations.

3.1. Basic properties. Various properties of LOFs can be found in [9]. For clarity, here we just list some useful results:

- *Orthogonality*: Owing to the orthogonality of Laguerre polynomials, there exists

$$\int_0^1 \mathcal{S}_n(t)\, \mathcal{S}_m(t)\, \mathrm{d}t = (\beta + 1)^{-1}\delta_{mn}, \quad t \in I := (0,1).$$

- *Gauss-LOFs quadrature*: Let $\{x_j,\ \omega_j\}_{j=0}^N$ be the Gauss nodes and weights of Laguerre polynomial $\mathscr{L}_{N+1}(x)$. Denote

$$\big\{t_j = e^{-x_j/(\beta+1)}, \quad \chi_j = \omega_j t_j^{-\beta}/(\beta+1)\big\}_{j=0}^N.$$

Then, for any $p \in \mathcal{P}_{2N+1}^{\beta,\log t}$, there exists

$$(3.1) \qquad \int_0^1 p(t)\mathrm{d}x = \sum_{j=0}^N p(t_j)\, \chi_j,$$

where the approximation space

$$\mathcal{P}_K^{\beta,\log t} := \mathrm{span}\{t^\beta,\ t^\beta \log t,\ t^\beta(\log t)^2, \ldots, t^\beta(\log t)^K\}.$$

- *Closed form*: The closed form can be read as

$$\mathcal{S}_n(t) = \sum_{k=0}^n \frac{(-1)^k}{k!}\binom{n}{n-k} t^{\frac{\beta}{2}}[-(\beta+1)\log t]^k.$$

In particular, $\mathcal{S}_n(1) = 1$.

- *Generalized derivative relation*: Define the generalized derivative

$$\partial_{\gamma,t} u := t^{\gamma+1}\partial_t\{t^{-\gamma}u\} = t\partial_t u - \gamma u.$$

For parameter $\gamma = \beta/2$, it holds that

$$\partial_{\gamma,t}\, \mathcal{S}_n(t) = \partial_{\frac{\beta}{2},t}\, \mathcal{S}_n(t) = (\beta+1)\sum_{l=0}^{n-1}\mathcal{S}_l(t).$$

Then, combining the above equalities, it holds that

$$\partial_t\, \mathcal{S}_n(t) = t^{-1}\bigg(\frac{\beta}{2}\mathcal{S}_n(t) + (\beta+1)\sum_{l=0}^{n-1}\mathcal{S}_l(t)\bigg).$$

3.2. Approximation properties by LOFs. Here we shall introduce the approximation properties of the LOFs, which will be intensively used in the subsequent section. To this end, we denote the L^2-projection $\Pi_N u$ from $L^2(I)$ to $\mathcal{P}_N^{\frac{\beta}{2},\log t}$ by satisfying

$$(3.2) \qquad \int_0^1 (u - \Pi_N u)v\, \mathrm{d}t = 0 \quad \forall v \in \mathcal{P}_N^{\frac{\beta}{2},\log t}.$$

Owing to the orthogonality of the LOFs, it holds that

$$\Pi_N u(t) = \sum_{n=0}^{N} \hat{u}_n \, \mathcal{S}_n(t), \quad \text{with} \quad \hat{u}_n = (\beta + 1) \int_0^1 u(t) \, \mathcal{S}_n(t) \, \mathrm{d}t.$$

Moreover, for describing the approximability of the projection $\Pi_N u$, we define the following nonuniformly weighted Sobolev space:

$$A_\gamma^m(I) := \{v \in L^2(I): \, \partial_{\gamma,t}^k v \in L_{\chi^k}^2(I), \, k = 1, 2, \ldots, m\}, \quad \text{with} \quad \chi(t) := |\log t|$$

equipped with seminorm and norm

$$|v|_{A_\gamma^m(I)} := \|\partial_{\gamma,t}^m v\|_{L_{\chi^m}^2(I)}, \quad \|v\|_{A_a^m(I)} := \left(\sum_{k=0}^{m} |v|_{A_a^k(I)}^2\right)^{1/2}.$$

Here $L_w^2(I)$ denotes the weighted $L^2(I)$ space with norm $\|u\|_{L_w^2(I)}^2 = \int_I |u(t)|^2 w(t) \, dt$.

LEMMA 3.1 (see [9, Theorem 2.1]). *Let m, N, $k \in \mathbb{N}$, and let $\beta > -1$. For any $u \in A_{\beta/2}^m(I)$ and $0 \le k \le \widetilde{m}$, $\widetilde{m} = \min\{m, N+1\}$, we have*

$$(3.3) \qquad |u - \Pi_N u|_{A_{\beta/2}^k(I)} \le \sqrt{\frac{(\beta+1)^{k-\widetilde{m}}(N-\widetilde{m}+1)!}{(N-k+1)!}} \, |u|_{A_{\beta/2}^{\widetilde{m}}(I)}.$$

In particular, for fixed $m < N$, there exists

$$(3.4) \qquad |u - \Pi_N u|_{A_{\beta/2}^k(I)} \le c N^{(k-m)/2} \, |u|_{A_{\beta/2}^m(I)},$$

where the constant c depends on β, k, and m.

3.3. Approximation to Mittag–Leffler functions. Recalling the solution representation given in (2.8) and Remark 2.1, the main part in the time direction consists of Mittag–Leffler functions $E_{\nu,1}(-\lambda t^\nu)$, which are weakly singular near $t = 0$. This fact leads to the ineffectiveness of many numerical methods for solving the subdiffusion model.

However, for any fixed integer m, it is easy to observe that for any $\beta > 0$ and $\nu \in (0, 1)$

$$\partial_{\frac{\beta}{2},t}^m E_{\nu,1}(-\lambda t^\nu) = \sum_{j=0}^{\infty} \frac{(\nu j - \frac{\beta}{2})^m}{\Gamma(\nu j + 1)} (-\lambda t^\nu)^j,$$

which is still in $C[0,1]$. Therefore, $E_{\nu,1}(-\lambda t^\nu) \in A_{\beta/2}^m(I)$ for any $\beta > 0$, and the bound of the seminorm is independent of λ. This observation together with the approximation properties given in Lemma 3.1 indicates that the Mittag–Leffler functions $E_{\nu,1}(-\lambda t^\nu)$ can be approximated efficiently by using LOFs and hence motivates us to use LOF spectral methods to solve the subdiffusion equation (2.6).

To see this, we test the approximation to the Mittag–Leffler function $E_{\nu,1}(-\lambda t^\nu)$ on the unit interval $I = (0, 1)$, using the LOFs $\{S_n(t; \beta)\}_{n=0}^N$ as basis functions. We evaluate the L^2-error

$$e_N = \|(\Pi_N - I)E_{\nu,1}(-\lambda t^\nu)\|_{L^2(I)}.$$

In Figure 1 (left), we plot the numerical error curves for different ν, where we fixed $\beta = 6$ and $\lambda = 5$. The numerical results demonstrate that the numerical approximation of LOFs exponentially converges to the Mittag–Leffler function. Moreover,
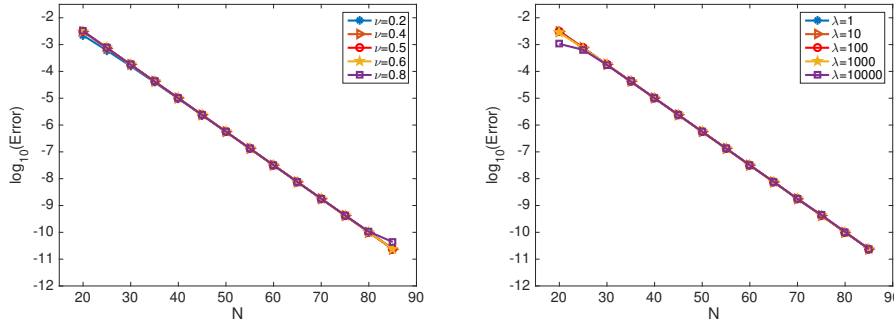
FIG. 1. *Left: plot of e_N for $E_{\nu,1}(-5t^\nu)$ with different ν. Right: plot of e_N for $E_{0.7,1}(-\lambda t^{0.7})$ with different λ.*

since the solution (2.8) consists of Mittag–Leffler functions with different eigenvalues $\lambda_1 < \lambda_2 < \cdots < \lambda_n < \cdots$, we also check the error e_N with different λ, in order to verify that LOFs are efficient for approximating Mittag–Leffler functions with a large eigenvalue. In Figure 1 (right), we draw the numerical error curves, with fixed $\beta = 6$ and $\nu = 0.7$, for different λ. Our numerical results show that the value of λ does not significantly affect the projection error which decays exponentially. Those numerical results indicate that the LOFs are suitable for approximating Mittag–Leffler functions with different parameters and hence also proper for solving fractional subdiffusion equation (2.6).

3.4. Shifted generalized LOFs. In the preceding section, we discussed the approximation to Mittag–Leffler functions on the unit interval by using the LOFs. Next, we shall consider the general interval $\Lambda = (0, T)$ and the solution of subdiffusion equation (2.6). To this end, with a slight modification, we define a new class of LOFs as

$$(3.5) \qquad \widehat{\mathcal{S}}_n^\nu(t) := (t/T)^{\frac{\nu}{2}} \mathcal{S}_n(t/T; \beta), \quad t \in (0, T),$$

and an L^2-projection $\widehat{\Pi}_N$ from $L^2(\Lambda)$ onto the space spanned by $\{\mathcal{S}_n(t/T)\}_{n=0}^N$ by

$$\widehat{\Pi}_N u(t) := \Pi_N u(T\tau), \quad \text{with} \quad \tau \in (0, 1).$$

Remark 3.1. The modified basis functions $\widehat{\mathcal{S}}_n^\nu(t)$ coincide with a special case of the shifted generalized LOFs (SGLOFs) [9]. The power functions $(t/T)^{\frac{\nu}{2}}$ multiplying the shifted LOFs $\mathcal{S}_n(t/T; \beta)$ is for the convenience of the error analysis. Hereafter, for simplicity, we still call the modified basis LOFs.

Besides, we shall also define the shifted weighted Sobolev space $A_{\gamma,T}^m(\Lambda)$:

$$A_{\gamma,T}^m(I) := \{v \in L^2(\Lambda) : \partial_{\gamma,t}^k v \in L_{\chi_T^k}^2(\Lambda), \ k = 1, 2, \ldots, m\}, \quad \text{with} \quad \chi_T(t) := |\log(t/T)|.$$

Then we have the following approximation properties of SGLOFs.

LEMMA 3.2. *Let $0 < \nu < 1$, $\beta > 0$, and $\Lambda = (0, T)$. For any $u \in H_0^{\frac{\nu}{2}}(\Lambda)$ and ${}_0\mathrm{D}_t^{\frac{\nu}{2}} u \in A_{\frac{\beta}{2},T}^m(\Lambda)$, the global-in-time projection*

$$\Pi_N^t u(t) := {}_0\mathrm{I}_t^{\frac{\nu}{2}} \widehat{\Pi}_N {}_0\mathrm{D}_t^{\frac{\nu}{2}} u$$

belongs to the linear vector space spanned by $\{\widehat{\mathcal{S}}_n^\nu\}_{n=0}^N$ and satisfying

$$(3.6) \qquad \|\Pi_N^t u - u\|_{H^{\frac{\nu}{2}}(\Lambda)} \le c\|_0\mathrm{D}_t^{\frac{\nu}{2}}(\Pi_N^t u - u)\|_{L^2(\Lambda)} \le cN^{-m/2}\ |_0\mathrm{D}_t^{\frac{\nu}{2}} u|_{A^m_{\frac{\beta}{2},T}(\Lambda)},$$

where the constant c depends on β, k, and m.

Proof. First of all, we note that for any $\nu \in (0,1)$ and $u \in H_0^{\frac{\nu}{2}}(\Lambda)$ it holds that $_0\mathrm{D}_t^{\frac{\nu}{2}} u \in L^2(\Lambda)$, and hence $\widehat{\Pi}_N(_0\mathrm{D}_t^{\frac{\nu}{2}} u)$ is well defined. Meanwhile, using the fact that $\nu \in (0,1)$, we know the fractional integral operator $_0\mathrm{I}_t^{\frac{\nu}{2}}$ is bounded from $L^2(\Lambda)$ to $H_0^{\frac{\nu}{2}}(\Lambda)$ [23, Theorems 2.1], and hence we have $\Pi_N^t u \in H^{\frac{\nu}{2}}(\Lambda)$. Then the first inequality is valid owing to the Poincaré inequality and the equivalence relation (2.2):

$$\|\Pi_N^t u - u\|_{H^{\frac{\nu}{2}}(\Lambda)} \le c|\Pi_N^t u - u|_{H_0^{\frac{\nu}{2}}(\Lambda)} \le c\|_0\mathrm{D}_t^{\frac{\nu}{2}}(\Pi_N^t u - u)\|_{L^2(\Lambda)}.$$

Next, for any v defined on Λ, we define $\widehat{v}(\tau) = v(T\tau)$, with $\tau \in I = (0,1)$. Then, owing to the approximation result given in (3.4), it holds that

$$\|(\widehat{\Pi}_N - I)v\|_{L^2(\Lambda)} = \sqrt{T}\|(\Pi_N - I)\widehat{v}\|_{L^2(I)} \le c\sqrt{T}N^{-m/2}\ |\widehat{v}|_{A^m_{\beta/2}(I)}.$$

Hence, we arrive at

$$(3.7) \qquad \|(\widehat{\Pi}_N - I)v\|_{L^2(\Lambda)} \le cN^{-m/2}\ \|v\|_{A^m_{\beta/2,T}(\Lambda)}.$$

Therefore, the claim (3.6) is valid. Then we shall prove that $\Pi_N^t u = {_0\mathrm{I}_t^{\frac{\nu}{2}}} \widehat{\Pi}_{N0}\mathrm{D}_t^{\frac{\nu}{2}} u$ can be expanded by SGLOFs $\{\widehat{\mathcal{S}}_n^\nu(t)\}_{n=1}^N$. In fact, due to the facts that

$$\mathrm{span}\{\widehat{\mathcal{S}}_n^\nu(t)\}_{n=0}^N = \mathrm{span}\{t^{\frac{\nu+\beta}{2}}(\log t)^k\}_{k=0}^N \quad \text{and} \quad \widehat{\Pi}_{N0}\mathrm{D}_t^{\frac{\nu}{2}} u = \sum_{n=0}^N a_n \widehat{\mathcal{S}}_n^0 = \sum_{k=0}^N a_n' t^{\frac{\beta}{2}}(\log t)^k,$$

it suffices to show that $_0\mathrm{I}_t^{\frac{\nu}{2}}\{t^{\frac{\beta}{2}}(\log t)^k\}_{k=0}^N$ belongs to $\mathrm{span}\{t^{\frac{\nu+\beta}{2}}(\log t)^k\}_{k=0}^N$. Now we observe that

$$
\begin{aligned}
_0\mathrm{I}_t^{\frac{\nu}{2}}\{t^{\frac{\beta}{2}}(\log t)^k\} &= \frac{1}{\Gamma(\frac{\nu}{2})}\int_0^t (t-\tau)^{\frac{\nu}{2}-1}\tau^{\frac{\beta}{2}}(\log\tau)^k\mathrm{d}\tau \\
&\overset{\tau=ts}{=} \frac{1}{\Gamma(\frac{\nu}{2})}\int_0^1 t^{\frac{\nu+\beta}{2}}(1-s)^{\frac{\nu}{2}-1}s^{\frac{\beta}{2}}(\log t + \log s)^k\mathrm{d}s \\
&= \sum_{j=0}^k t^{\frac{\nu+\beta}{2}}(\log t)^j \frac{1}{\Gamma(\frac{\nu}{2})}\int_0^1 (1-s)^{\frac{\nu}{2}-1}s^{\frac{\beta}{2}}\binom{k}{j}(\log s)^k\mathrm{d}s.
\end{aligned}
$$

Finally, the estimate (3.6) can be derived by using (3.7). $\qquad\square$

4. Spectral-Galerkin method for subdiffusion equations. In this section, we shall develop a spectral-Galerkin method for solving the subdiffusion equation (2.6) with rigorous analysis. A fully discrete scheme based on a finite element method in space and a fast algorithm to solve the matrix system will also be provided.

4.1. Wellposedness of the weak problem. In order to solve the subdiffusion equation, we follow the standard space-time Galerkin framework. To this end, we define a space-time Hilbert space

$$H_0^{s,1}(\mathcal{O}) := H_0^s\big(\Lambda; L^2(\Omega)\big) \cap L^2\big(\Lambda; H_0^1(\Omega)\big), \quad \mathcal{O} := \Lambda \times \Omega,$$

endowed with the norm

$$\|v\|_{H_0^{s,1}(\mathcal{O})} := \left(\|v\|_{H^s(\Lambda;L^2(\Omega))}^2 + \|v\|_{L^2(\Lambda;H^1(\Omega))}^2 \right)^{1/2}.$$

Recalling the assumptions on the elliptic operator L in (1.2), it induces a coercive bilinear form

$$a(u,v) = -(a\nabla u, \nabla v)_\Omega + (bu, v)_\Omega \quad \forall u, v \in H_0^1(\Omega),$$

which satisfies

$$(4.1) \quad a(u,u) \geq c_1 \|u\|_{\dot{H}^1(\Omega)}^2 \quad \text{and} \quad a(u,v) \leq c_2 \|u\|_{\dot{H}^1(\Omega)} \|v\|_{\dot{H}^1(\Omega)} \quad \forall u, v \in H_0^1(\Omega).$$

Then a weak formulation of the subdiffusion equation (2.6) reads as follows: find $u \in H_0^{\frac{\nu}{2},1}(\mathcal{O})$ such that

$$(4.2) \qquad\qquad \mathcal{B}(u,v) = \mathcal{F}(v) \quad \forall v \in H_0^{\frac{\nu}{2},1}(\mathcal{O}),$$

where the bilinear form $\mathcal{B}(\cdot, \cdot)$ and the functional $\mathcal{F}(\cdot)$ are respectively defined by

$$\mathcal{B}(u,v) := \int_0^T \left({}_0\mathrm{D}_t^{\frac{\nu}{2}} u \,, {}_t\mathrm{D}_T^{\frac{\nu}{2}} v \right)_\Omega + a\big(u,v\big) \, \mathrm{d}t, \qquad \mathcal{F}(v) := \int_0^T (f,v)_\Omega \, \mathrm{d}t.$$

LEMMA 4.1. *For any $u, v \in H_0^{\frac{\nu}{2},1}(\mathcal{O})$, there exist constants c_1, c_2 such that*

$$(4.3) \qquad \mathcal{B}(u,u) \geq c_1 \|u\|_{H_0^{\frac{\nu}{2},1}(\mathcal{O})}, \quad \mathcal{B}(u,v) \leq c_2 \|u\|_{H_0^{\frac{\nu}{2},1}(\mathcal{O})} \|v\|_{H_0^{\frac{\nu}{2},1}(\mathcal{O})}.$$

Proof. The coercivity and continuity of the bilinear form $\mathcal{B}(\cdot, \cdot)$ are the straightforward results from the elliptic conditions (4.1), the Cauchy–Schwarz inequality, the properties (2.2) and (2.4), and the fractional Poincaré inequality. □

With the elliptic conditions (4.3) in hand, we can claim the wellposedness of the weak formulation of the subdiffusion equation by the Lax–Milgram lemma as follows.

THEOREM 4.2. *Let there be a function f belonging to $\left(H_0^{\frac{\nu}{2},1}(\mathcal{O})\right)'$, the dual space of $H_0^{\frac{\nu}{2},1}(\mathcal{O})$. For any $\nu \in (0,1)$, the weak problem (4.2) admits a unique solution u satisfying*

$$\|u\|_{H_0^{\frac{\nu}{2},1}(\mathcal{O})} \leq c\|f\|_{\left(H_0^{\frac{\nu}{2},1}(\mathcal{O})\right)'}.$$

4.2. Spectral-Galerkin method and error estimation. In this section, we shall develop and study a semidiscrete spectral-Galerkin method using the basis $\widehat{\mathcal{S}}_m^\nu(t)$ defined in (3.5). Here we define $X_N^t(\Lambda)$ to be a finite-dimensional subspace of $H_0^{\frac{\nu}{2}}(\Lambda)$,

$$(4.4) \qquad\qquad X_N^t = \mathrm{span}\{\widehat{\mathcal{S}}_n^\nu(t)\}_{n=0}^N,$$

which is a finite-dimensional subspace of $H_0^{\frac{\nu}{2}}(\Lambda)$. Then the semidiscrete-in-time scheme reads as follows: find $u_N \in V_N = X_N^t \otimes H_0^1(\Omega)$ such that

$$(4.5) \qquad\qquad \mathcal{B}(u_N, v) = \mathcal{F}(v) \quad \forall v \in V_N.$$

By the Lax–Milgram lemma, for any given function f belonging to $\left(H_0^{\frac{\nu}{2},1}(\mathcal{O})\right)'$, the semidiscrete problem admits a unique solution u_N satisfying

$$(4.6) \qquad\qquad \|u_N\|_{H_0^{\frac{\nu}{2},1}(\mathcal{O})} \leq c\|f\|_{\left(H_0^{\frac{\nu}{2},1}(\mathcal{O})\right)'}.$$

Next, we shall derive the error estimate for the semidiscrete solution. The error $u - u_N$ satisfies the Galerkin orthogonality

$$\mathcal{B}(u_N - u, v) = 0 \qquad \forall v \in V_N.$$

Recalling that $\Pi_N^t u \in V_N$ (by Lemma 3.2), the standard argument leads to

$$(4.7) \quad \|u_N - u\|_{H_0^{\frac{\nu}{2},1}(\mathcal{O})} \le c\|\Pi_N^t u - u\|_{H_0^{\frac{\nu}{2},1}(\mathcal{O})} \le c\|_0 D_t^{\frac{\nu}{2}} (\Pi_N^t u - u)\|_{L^2(\Lambda;H^1(\Omega))}.$$

To derive the error estimate, we shall use the following regularity estimate.

THEOREM 4.3. *Let u be the solution of the subdiffusion equation* (2.6). *For $k = 0, 1, \ldots, m$, if the source term f satisfies*

$$\partial_t^j(t^j f) \in L^2_{\chi_T^k}(\Lambda; H_0^1(\Omega)) \qquad \forall 0 \le j \le k,$$

then the solution u satisfies

$$\partial_{\gamma,t}^k(_0 D_t^{\frac{\nu}{2}} u) \in L^2_{\chi_T^k}(\Lambda; H_0^1(\Omega)), \quad k = 0, 1, \ldots, m,$$

where $\partial_{\gamma,t} := t\partial_t - \gamma$, with $\gamma > 0$ being a generalized derivative.

Proof. For a given suitable function $g(t)$, we have

$$
\begin{aligned}
_0 D_t^{\frac{\nu}{2}} & \int_0^t (t-\tau)^{\nu-1} E_{\nu,\nu}(-\lambda_n(t-\tau)^\nu) g(\tau) \mathrm{d}\tau \\
&= \frac{1}{\Gamma(1-\frac{\nu}{2})} \partial_t \int_0^t (t-s)^{-\frac{\nu}{2}} \int_0^s (s-\tau)^{\nu-1} E_{\nu,\nu}(-\lambda_n(s-\tau)^\nu) g(\tau) \, \mathrm{d}\tau \, \mathrm{d}s \\
&= \frac{1}{\Gamma(1-\frac{\nu}{2})} \partial_t \int_0^t g(\tau) \int_\tau^t (t-s)^{-\frac{\nu}{2}} (s-\tau)^{\nu-1} E_{\nu,\nu}(-\lambda_n(s-\tau)^\nu) \, \mathrm{d}s \, \mathrm{d}\tau \\
&= \partial_t \int_0^t (t-\tau)^{\frac{\nu}{2}} E_{\nu,1+\frac{\nu}{2}}(-\lambda_n(t-\tau)^\nu) \, g(\tau) \, \mathrm{d}\tau,
\end{aligned}
$$

(4.8)

where the validation of the last equality owes to

$$
\begin{aligned}
\int_\tau^t & (t-s)^{-\frac{\nu}{2}} (s-\tau)^{\nu-1} E_{\nu,\nu}(-\lambda_n(s-\tau)^\nu) \, \mathrm{d}s \\
&= (t-\tau)^{\frac{\nu}{2}} \int_0^1 (1-\theta)^{-\frac{\nu}{2}} \theta^{\nu-1} \sum_{j=0}^\infty \frac{(-\lambda_n)^j \theta^{j\nu}(t-\tau)^{j\nu}}{\Gamma(j\nu+\nu)} \, \mathrm{d}\theta \\
&= (t-\tau)^{\frac{\nu}{2}} \sum_{j=0}^\infty \frac{(-\lambda_n)^j (t-\tau)^{j\nu}}{\Gamma(j\nu+\nu)} \int_0^1 (1-\theta)^{-\frac{\nu}{2}} \theta^{j\nu+\nu-1} \, \mathrm{d}\theta \\
&= \Gamma\left(1 - \frac{\nu}{2}\right)(t-\tau)^{\frac{\nu}{2}} E_{\nu,1+\frac{\nu}{2}}(-\lambda_n(t-\tau)^\nu).
\end{aligned}
$$

(4.9)

Using the solution representation (2.8) and the derivative relation (2.7), it holds that

$$
\begin{aligned}
_0 D_t^{\frac{\nu}{2}} u(x,t) &= \sum_{n=1}^\infty \varphi_n(x) \, \partial_t \int_0^t (t-\tau)^{\frac{\nu}{2}} E_{\nu,1+\frac{\nu}{2}}(-\lambda_n(t-\tau)^\nu) \big(f(\cdot,\tau), \varphi_n\big)_\Omega \mathrm{d}\tau \\
&= \sum_{n=1}^\infty \varphi_n(x) \int_0^t (t-\tau)^{\frac{\nu}{2}-1} E_{\nu,\frac{\nu}{2}}(-\lambda_n(t-\tau)^\nu) \big(f(\cdot,\tau), \varphi_n\big)_\Omega \mathrm{d}\tau.
\end{aligned}
$$

(4.10)

Then we can rewrite $_0\mathrm{D}_t^{\frac{\nu}{2}} u$ as

(4.11)
$$_0\mathrm{D}_t^{\frac{\nu}{2}} u(t) = \int_0^t \bar{E}(t-\tau) f(\tau)\, \mathrm{d}\tau, \quad \text{where} \quad \bar{E}(t)v = \sum_{n=1}^{\infty} t^{\frac{\nu}{2}-1} E_{\nu,\frac{\nu}{2}}(-\lambda_n t^\nu)\big(v,\varphi_n\big)_\Omega \varphi_n.$$

Now we are ready to prove that $\partial_{\gamma,t}^k [_0\mathrm{D}_t^{\frac{\nu}{2}}(\Delta^{\frac{1}{2}} u)] \in L_{\chi_T^k}^2(\Lambda; L^2(\Omega))$. Thanks to the definition of the generalized derivative $\partial_{\gamma,t} = t\partial_t - \gamma$, we only need to check that $\partial_t^k\big(t^k[_0\mathrm{D}_t^{\frac{\nu}{2}}(\Delta^{\frac{1}{2}} u)]\big) \in L_{\chi_T^k}^2(\Lambda; L^2(\Omega))$ for $k = 0, 1, \ldots, m$. For this purpose, we observe that

$$\partial_t^k\big(t^k[_0\mathrm{D}_t^{\frac{\nu}{2}}(\Delta^{\frac{1}{2}} u)]\big)(t) = \partial_t^k\bigg(t^k \int_0^t \bar{E}(t-\tau)\Delta^{\frac{1}{2}} f(\tau)\, \mathrm{d}\tau\bigg)$$

$$= \sum_{j=0}^k \binom{k}{j} \partial_t^k\bigg(\int_0^t (t-\tau)^{k-j} \bar{E}(t-\tau)\, \tau^j f(\tau)\mathrm{d}\tau\bigg)$$

$$= \sum_{j=0}^k \binom{k}{j} \int_0^t \Big(\partial_t^{k-j}[(t-\tau)^{k-j}\bar{E}(t-\tau)]\Big) \Big(\partial_\tau^j[\tau^j \Delta^{\frac{1}{2}} f(\tau)]\Big)\mathrm{d}\tau.$$

The last equality holds due to the fact that

$$\lim_{t\to 0} t^{k+1}\partial_t^k f(t) = 0 \quad \text{and} \quad \lim_{t\to 0} t^{k+1}\partial_t^k \bar{E}(t)v = 0 \quad \forall v \in L^2(\Omega).$$

Thanks to Lemma 4.4, we have

$$\|\partial_t^k\big(t^k[_0\mathrm{D}_t^{\frac{\nu}{2}}(\Delta^{\frac{1}{2}} u)]\big)(t)\|_{L^2(\Omega)} \le c \sum_{j=0}^k \int_0^t (t-\tau)^{\frac{\nu}{2}-1}\|\partial_\tau^j[\tau^j \Delta^{\frac{1}{2}} f(\tau)]\|_{L^2(\Omega)}\, \mathrm{d}\tau =: c \sum_{j=0}^k K_j(t).$$

By Young's convolution inequality, we have

$$\int_0^T |K_j(t)|^2 |\log(t/T)|^k\, dt = \int_0^T \bigg|\int_0^t (t-\tau)^{\frac{\nu}{2}-1}\|\partial_\tau^j[\tau^j \Delta^{\frac{1}{2}} f(\tau)]\|_{L^2(\Omega)}\, \mathrm{d}\tau\bigg|^2 |\log(t/T)|^k\, dt$$

$$\le \int_0^T \bigg|\int_0^t (t-\tau)^{\frac{\nu}{2}-1}\Big(\|\partial_\tau^j[\tau^j \Delta^{\frac{1}{2}} f(\tau)]\|_{L^2(\Omega)}|\log(\tau/T)|^{\frac{k}{2}}\Big)\mathrm{d}\tau\bigg|^2\, dt$$

$$\le \bigg(\int_0^T t^{\frac{\nu}{2}-1}\, \mathrm{d}t\bigg)^2 \int_0^T \|\partial_\tau^j[\tau^j \Delta^{\frac{1}{2}} f(\tau)]\|_{L^2(\Omega)}^2 |\log(\tau/T)|^k\, dt$$

$$\le c \int_0^T \|\partial_\tau^j[\tau^j f(\tau)]\|_{H^1(\Omega)}^2 |\log(\tau/T)|^k\, dt \le c.$$

Therefore, $\partial_t^k\big(t^k[_0\mathrm{D}_t^{\frac{\nu}{2}} u]\big) \in L_{\chi_T^k}^2(\Lambda; H_0^1(\Omega))$ for $k = 0, 1, \ldots, m$, and so does $\partial_{\gamma,t}^k[_0\mathrm{D}_t^{\frac{\nu}{2}} u]$. This completes the proof of this theorem.   □

LEMMA 4.4. *Let $\bar{E}(t)$ be the operator defined in (4.11). Then it holds that*

$$\|\partial_t^k(t^k \bar{E}(t))v\|_{L^2(\Omega)} \le ct^{\frac{\nu}{2}-1}\|v\|_{L^2(\Omega)} \quad \forall v \in L^2(\Omega) \quad and \quad k = 0, 1, 2, \ldots,$$

where $\partial_t^k := \frac{\mathrm{d}^k}{\mathrm{d}t^k}$ is the k-fold derivative with respect to t.

Proof. Using the identity (2.7), we have

$$\partial_t^k(t^k \bar{E}(t))v = \sum_{j=0}^{k}\binom{k}{j}\sum_{n=1}^{\infty}(\partial_t^{k-j}t^k)\partial_t^j\left(t^{\frac{\nu}{2}-1}E_{\nu,\frac{\nu}{2}}(-\lambda_n t^\nu)\right)(v,\varphi_n)_\Omega \varphi_n$$

$$= \sum_{j=0}^{k}\frac{k!}{j!}\binom{k}{j}\sum_{n=1}^{\infty}t^{\frac{\nu}{2}-1}E_{\nu,\frac{\nu}{2}-j}(-\lambda_n t^\nu)(v,\varphi_n)_\Omega \varphi_n.$$

This together with Lemma 2.2 leads to

$$\|\partial_t^k(t^k\bar{E}(t))v\|_{L^2(\Omega)}^2 \le c\sum_{j=0}^{k}\sum_{n=1}^{\infty}\left|t^{\frac{\nu}{2}-1}E_{\nu,\frac{\nu}{2}-j}(-\lambda_n t^\nu)\right|^2(v,\varphi_n)_\Omega^2 \le ct^{\nu-2}\|v\|_{L^2(\Omega)}^2,$$

which completes the proof.   □

Combining (4.7) and Theorem 4.3 with the approximation properties stated in Lemma 3.2, we immediately obtain the following error estimate.

THEOREM 4.5. *Let u be the solution of the subdiffusion equation* (2.6) *and u_N be the semidiscrete solution of the spectral-Galerkin scheme* (4.5). *If the source term f satisfies*

$$\partial_t^j(t^j f) \in L^2_{\chi_T^k}(\Lambda; H_0^1(\Omega)) \quad \forall 0 \le j \le k \quad and \quad k = 0, 1, \ldots, m,$$

then it holds that

$$\|u_N - u\|_{H_0^{\frac{\nu}{2},1}(\mathcal{O})} \le cN^{-m/2}.$$

Here the constant is independent of N and u but may depend on $\nu, \beta, m, T,$ and f.

Remark 4.1. In case that the initial condition of the subdiffusion problem is not zero, we may derive the same result by assuming that $u_0 \in \dot{H}^3(\Omega)$. Recall that the initial value $u_0(x)$ of the subdiffusion equation (1.1) transforms to Lu_0 arising in the source term in (2.6), and it is easy to verify that $\partial_t^n(t^n Lu_0) \in C^\infty([0,T];H_0^1(\Omega))$ for any positive integer n.

Remark 4.2. In Jin, Lazarov, and Zhou [25] and Jin, Li, and Zhou [27], the authors developed time-stepping schemes using convolution quadrature generated by high-order BDF methods, motivated by the pioneer work in [39, 12]. An initial correction strategy was proposed to restore high-order convergence. See also [63] for the analysis of the $L1$ scheme with initial correction and [16, 5] for the convolution quadrature Runge–Kutta schemes. One requirement of those time-stepping schemes in the aforementioned works is that the source term f needs to be smooth in the time direction. As an example, the kth-order BDF method requires $f \in W^{k,1}((0,T);L^2(\Omega)) \cap f \in W^{k,\infty}((\epsilon,T);L^2(\Omega))$, and the high-order convergence will deteriorate if f is not regular enough (cf. [27, section 4]). Therefore, it is nontrivial to extend the strategy and analysis to nonlinear problems [28] or problems with time-dependent diffusion coefficients [26, 29]. Compared with those schemes, the spectral Galerkin method (4.5) allows singularity of the source term near $t = 0$, and hence also performs well for solving linear subdiffusion equations with time-dependent diffusion coefficients as well as nonlinear subdiffusion problems. See section 5 for numerical results and more discussion. On the other hand, the spectral Galerkin method requires a smooth initial condition, and the error estimate was derived in the space-time energy

norm, while the time-stepping schemes in [25, 27] lead to an optimal pointwise-in-time error estimate at a fixed time (even for nonsmooth initial data $u_0 \in L^2(\Omega)$). How to derive a pointwise-in-time error estimate for the spectral Galerkin method (4.5) requires further investigation.

4.3. Fully discrete scheme and error estimation. In this section, we shall discuss the fully discrete scheme based on our preceding results. As an example, we apply the $P1$ conforming finite element in space. Here we introduce a quasi-uniform shape regular partition of the domain Ω into simplicial elements of maximal diameter h, which is denoted by $\mathcal{T}_h$. We consider the space of continuous piecewise linear functions on $\mathcal{T}_h$ with $N \in \mathbb{N}$ being the number of degrees of freedom. Let $\{\varphi_i\}_{i=1}^M \subset H_0^1(\Omega)$ be the nodal basis functions, and denote

$$(4.12) \qquad X_h^x := \operatorname{span}\{\varphi_i\}_{i=1}^M.$$

The L^2-projection $P_h : L^2(\Omega) \to X_h^x$ is defined by

$$(\phi - P_h\phi, v)_\Omega = 0 \quad \forall v \in X_h^x.$$

It is well known that it satisfies the following error estimate [59]:

$$(4.13)$$
$$\|P_h\phi - \phi\|_{L^2(\Omega)} + h\|\nabla(P_h\phi - \phi)\|_{L^2(\Omega)} \le ch^q \|\phi\|_{H^q(\Omega)} \quad \forall \phi \in H_0^1(\Omega) \cap H^q(\Omega), \ q = 1, 2.$$

Then the spatially semidiscrete scheme reads as follows: find $u_h \in W_h = H_0^{\frac{\nu}{2}}(0,T) \otimes X_h^x$ such that

$$(4.14) \qquad \mathcal{B}(u_h, v) = \mathcal{F}(v) \quad \forall v \in W_h.$$

The wellposedness follows from the coercivity of the bilinear form and the Lax–Milgram lemma.

Upon introducing the discrete operator $L_h : X_h^x \to X_h^x$ defined by $-(L_h\psi, \chi) = a(\psi, \chi)$ for all $\psi, \chi \in X_h$, let $\{\lambda_j^h, \varphi_j^h\}_{j=1}^N$ be the eigenpairs of the discrete operator $-L_h$. Now we introduce the discrete analogue E_h of the operator E defined in (2.8) for $t > 0$ and $v_h \in X_h$:

$$(4.15) \qquad E_h(t)v_h = \sum_{j=1}^N t^{\nu-1} E_{\nu,\nu}(-\lambda_j^h t^\nu)\,(v_h, \varphi_j^h)_\Omega\,\varphi_j^h.$$

Then the solution $u_h(t)$ of the spatially semidiscrete problem (4.14) can be represented by [24, equation (3.4)]

$$(4.16) \qquad u_h(t) = \int_0^t E_h(t-s)P_h f(s)\,ds.$$

LEMMA 4.6. *For $f \in L^2(\Lambda; L^2(\Omega))$, the spatially semidiscrete solution u_h in (4.14) satisfies*

$$\|u_h - u\|_{H_0^{\frac{\nu}{2},1}(\mathcal{O})} \le ch\|f\|_{L^2(\Lambda;L^2(\Omega))}.$$

Proof. By the approximation property (4.13), we have for $\varrho = P_h u - u$

$$\|\varrho\|_{H_0^{\frac{\nu}{2},1}(\mathcal{O})}^2 = \|\varrho\|_{H_0^{\frac{\nu}{2}}(\Lambda;L^2(\Omega))}^2 + \|\nabla\varrho\|_{L^2(\Lambda;L^2(\Omega))}^2$$
$$\le ch^2\Big(\|\nabla u\|_{H_0^{\frac{\nu}{2}}(\Lambda;L^2(\Omega))}^2 + \|u\|_{L^2(\Lambda;H^2(\Omega))}^2\Big).$$

Then by applying (2.2), (2.3), and regularity results [24, Theorem 2.1], we obtain

$$\|\nabla u\|^2_{H_0^{\frac{\nu}{2}}(\Lambda;L^2(\Omega))} \le c \int_0^T \left({}_0\mathrm{D}_t^{\frac{\nu}{2}}\nabla u\,,{}_t\mathrm{D}_T^{\frac{\nu}{2}}\nabla u\right)_\Omega \mathrm{d}t = c\int_0^T \left({}_0\mathrm{D}_t^{\nu}u\,,-\Delta u\right)_\Omega \mathrm{d}t$$
$$\le c\|{}_0\mathrm{D}_t^{\nu}u\|^2_{L^2(\Lambda;L^2(\Omega))} + c\|\Delta u\|^2_{L^2(\Lambda;L^2(\Omega))} \le c\|f\|^2_{L^2(\Lambda;L^2(\Omega))}.$$

Therefore, we arrive at

$$(4.17) \qquad \|\varrho\|_{H_0^{\frac{\nu}{2},1}(\mathcal{O})} \le ch\|f\|_{L^2(\Lambda;L^2(\Omega))}.$$

The function $\vartheta := u_h - P_h u$ satisfies $\vartheta(0) = 0$ and ${}_0\partial_t^\alpha \vartheta - L_h\vartheta = L_h(P_h u - R_h u) = L_h R_h \varrho$ (with R_h being the Ritz projection) [24, equation (3.9)]. By the regularity results, we have

$$\|\vartheta\|_{H^\nu(\Lambda;H^{-1}(\Omega))} + \|\vartheta\|_{L^2(\Lambda;H_0^1(\Omega))} \le c\|L_h R_h \varrho\|_{L^2(0,T;H^{-1}(\Omega))}.$$

Then the interpolation between $H^\nu(\Lambda;H^{-1}(\Omega))$ and $L^2(\Lambda;H_0^1(\Omega))$ yields that (note that $\frac{\nu}{2} < \frac{1}{2}$)

$$\|\vartheta\|_{H_0^{\frac{\nu}{2}}(\Lambda;L^2(\Omega))} + \|\vartheta\|_{L^2(\Lambda;H_0^1(\Omega))} \le c\|L_h R_h \varrho\|_{L^2(\Lambda;H^{-1}(\Omega))}.$$

This together with the estimate (4.17) leads to
$$(4.18)$$
$$\|\vartheta\|_{H_0^{\frac{\nu}{2},1}(\mathcal{O})} \le c\|L_h R_h \varrho\|_{L^2(\Lambda;H^{-1}(\Omega))} \le c\|\nabla R_h \varrho\|_{L^2(\Lambda;L^2(\Omega))} \le ch\|f\|_{L^2(\Lambda;L^2(\Omega))}.$$

As a result, (4.17), (4.18), and the triangle inequality complete the proof. □

The next lemma, which is an analogue to Theorem 4.3, provides regularity results of u_h in the time direction. The proof, relying on the solution representation (4.16) and the property of Mittag–Leffler functions, is similar to the proof of Theorem 4.3. The details can be found in Appendix B.

LEMMA 4.7. *Let u_h be spatially semidiscrete solution in* (4.14). *For $k = 0, 1, \ldots, m$, if the source term f satisfies*

$$\partial_t^j(t^j f) \in L^2_{\chi_T^k}(\Lambda;H_0^1(\Omega)) \quad \forall 0 \le j \le k,$$

then the solution u satisfies

$$\partial_{\gamma,t0}^k \mathrm{D}_t^{\frac{\nu}{2}} u_h \in L^2_{\chi_T^k}(\Lambda;H_0^1(\Omega)) \quad for \quad k = 0, 1, \ldots, m,$$

where $\partial_{\gamma,t} := t\partial_t - \gamma$, with $\gamma > 0$ being a generalized derivative.

Now we are ready to develop a fully discrete scheme. Let $X_N^t(\Lambda)$ and $X_h^x(\Omega)$ be finite-dimensional spaces defined in (4.4) and (4.12), respectively. Then the fully discrete scheme reads as follows: find $u_{hN} \in X_{hN} := X_N^t \otimes X_h^x$ such that

$$(4.19) \qquad \mathcal{B}(u_{hN},v) = (f,v) \quad \forall v \in X_{hN}.$$

Similarly, the wellposedness of the above numerical scheme can be guaranteed by the coercivity of linear form $\mathcal{B}(\cdot,\cdot)$ and the Lax–Milgram lemma.

The following theorem provides an estimate on the difference between the fully discrete solution u_{hN} and the spatially semidiscrete solution u_h.

THEOREM 4.8. *Let u_h be the solution of the spatially semidiscrete scheme (4.14) and u_{hN} be the fully discrete solution satisfying (4.19). If the resource term f satisfies*

$$\partial_t^j(t^j f) \in L^2_{\chi_T^k}(\Lambda; H_0^1(\Omega)) \quad \forall 0 \le j \le k \quad and \quad k = 0, 1, \dots, m,$$

then it holds that

$$\|u_{hN} - u_h\|_{H_0^{\frac{\nu}{2},1}(\mathcal{O})} \le c_2 N^{-m/2}.$$

Here the constant is independent of h, N, and u but may depend on ν, β, m, T, and f.

To estimate the numerical error $u_{hN} - u$, we split it into two components:

$$u_{hN} - u = (u_{hN} - u_h) + (u_h - u).$$

Note that the bound of $u_h - u$ and $u_{hN} - u_h$ has already been established in Theorems 4.5 and 4.8, respectively.

COROLLARY 4.9. *Let u be the solution of the subdiffusion equation (2.6) and u_{hN} be the fully discrete solution satisfying (4.19). If the resource term $f \in L^2(\Lambda; L^2(\Omega))$ also satisfies*

$$\partial_t^j(t^j f) \in L^2_{\chi_T^k}(\Lambda; H_0^1(\Omega)) \quad \forall 0 \le j \le k \quad and \quad k = 0, 1, \dots, m,$$

then it holds that

$$\|u_{hN} - u\|_{H_0^{\frac{\nu}{2},1}(\mathcal{O})} \le c_1 h + c_2 N^{-m/2}.$$

Here the constant is independent of h, N, and u, but c_1 may depend on ν, f, and T, and c_2 may depend on ν, β, m, T, and f.

4.4. Fast solver. In this section, we want to develop a fast algorithm to solve the space-time linear system (4.19). By substituting $u_{hN} = \sum_{m=1}^{M} \sum_{n=0}^{N} \tilde{u}_{mn} \phi_m(x) \widehat{\mathcal{S}}_n^\nu(t)$ and $v = \phi_p(x) \widehat{\mathcal{S}}_q^\nu(t)$, $p = 1, \dots, M$, $q = 0, 1, \dots, N$, the fully discrete scheme (4.19) is equivalent to solving the following matrix system:

$$(4.20) \qquad \mathbf{S}^x \mathbf{U} (\mathbf{M}^t)^T + \mathbf{M}^x \mathbf{U} (\mathbf{S}^t)^T = \mathbf{F},$$

where $\mathbf{M}^x$ and $\mathbf{S}^x$ are the mass and stiffness matrices in the x-direction(s), and $\mathbf{M}^t$ and $\mathbf{S}^t$ are the mass and stiffness matrices in the t-direction below:

$$
\begin{aligned}
\mathbf{S}^x &= (s_{pm}^x), & s_{pm}^x &= \left(L\phi_m, \phi_p\right)_\Omega; & \mathbf{M}^x &= (m_{pm}^x), & m_{ml}^x &= \left(\phi_m, \phi_p\right)_\Omega, \\
\mathbf{S}^t &= (s_{qn}^t), & s_{qn}^t &= \left({}_0\mathrm{D}_t^{\frac{\nu}{2}} \widehat{\mathcal{S}}_n^\nu, {}_t\mathrm{D}_T^{\frac{\nu}{2}} \widehat{\mathcal{S}}_q^\nu\right)_\Lambda, & \mathbf{M}^t &= (m_{qn}^t), & m_{pn}^t &= \left(\widehat{\mathcal{S}}_n^\nu, \widehat{\mathcal{S}}_q^\nu\right)_\Lambda, \\
\mathbf{U} &= (u_{mn}), & u_{mn} &= \tilde{u}_{mn}, & \mathbf{F} &= (f_{pq}), & f_{pq} &= \left(f, \phi_p \widehat{\mathcal{S}}_q^\nu\right).
\end{aligned}
$$

Notice that both the matrices $\mathbf{M}^t$ and $\mathbf{S}^t$ are nonsymmetric (see Appendix A), so the classical matrix diagonalization method [40, 17, 52] cannot be applied directly. To overcome this difficulty, we shall apply an efficient QZ decomposition method recently proposed by Shen and Sheng [54].

The key point of the new method is the following QZ decomposition:

$$\mathbf{Q}(\mathbf{S}^t)^T \mathbf{Z} = \mathbf{A}, \quad \mathbf{Q}(\mathbf{M}^t)^T \mathbf{Z} = \mathbf{B},$$

where $\mathbf{Q}$, $\mathbf{Z}$ are unitary matrices satisfying $\mathbf{QQ}^T = \mathbf{ZZ}^T = \mathbf{I}$, and $\mathbf{A}$, $\mathbf{B}$ are upper triangular matrices, namely,

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \ldots & a_{1N} \\ & a_{22} & \ldots & a_{2N} \\ & & \ddots & \vdots \\ & & & a_{NN} \end{pmatrix}, \qquad \mathbf{B} = \begin{pmatrix} b_{11} & b_{12} & \ldots & b_{1N} \\ & b_{22} & \ldots & b_{2N} \\ & & \ddots & \vdots \\ & & & b_{NN} \end{pmatrix}.$$

Then, by setting $\mathbf{U} = \mathbf{VQ}$ and multiplying (4.20) by both sides of $\mathbf{Z}$, we have an equivalent form

$$(4.21) \qquad \mathbf{M}^x \mathbf{V} \mathbf{A} + \mathbf{S}^x \mathbf{V} \mathbf{B} = \mathbf{G} := \mathbf{FZ}.$$

Denote by $\mathbf{v}_n = (v_{1n}, v_{2n}, \ldots, v_{Mn})^T$ the nth column of the matrix $\mathbf{V}$, i.e.,

$$\mathbf{V} = [\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N] = \begin{pmatrix} v_{11} & v_{12} & \ldots & v_{1N} \\ v_{21} & v_{22} & \ldots & v_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ v_{M1} & v_{M2} & \ldots & v_{MN} \end{pmatrix}.$$

The matrix system (4.21) can be solved by the following fast algorithm:

$$(4.22) \qquad \left(a_{nn}\mathbf{M}^x + b_{nn}\mathbf{S}^x\right) \mathbf{v}_n = \mathbf{g}_n - \mathbf{h}_{n-1}, \quad n = 1, 2, \ldots, N,$$

where $\mathbf{g}_n$ is the nth column of the matrix $\mathbf{G}$ and

$$\mathbf{h}_0 = \mathbf{0}, \quad \mathbf{h}_{n-1} = \mathbf{M}^x \left(\sum_{k=1}^{n-1} a_{kn} \mathbf{v}_k \right) + \mathbf{S}^x \left(\sum_{k=1}^{n-1} b_{kn} \mathbf{v}_k \right).$$

Note that the new algorithm (4.22) is indeed equivalent to solving the following N times elliptical problems:

$$-a_{nn}Lv(x) + b_{nn}v(x) = g_h(x), \quad n = 1, 2, \ldots, N.$$

As shown in Theorem 4.8, our scheme enjoys spectral convergence in time, so in general only small N is needed to achieve the desired accuracy. On the other hand, the above elliptic problems can be solved efficiently by usual multigrid or other fast solvers. Therefore, our space-time scheme is very efficient.

5. Numerical experiments, extensions, and discussions. In this section, we present some numerical examples to illustrate our theoretical results proposed in previous sections, and in addition we apply the proposed techniques to problems with time-dependent diffusion coefficients and to a nonlinear time-fractional Allen–Cahn equation. In our experiments, we computed the numerical solutions of the fully discrete scheme (4.19), with the spectral-Galerkin method in time and the Galerkin finite element method in space. Since the spatially semidiscrete solution has been verified in [24], we focus on the temporal discretization error below. All the computations are carried out in MATLAB R2015a on a personal laptop.

Example (a). Subdiffusion problems with time-independent coefficients. In the first example, we present the numerical results for the following two dimension subdiffusion problem on the unit square domain $\Omega = (0,1)^2$. Letting $0 < \nu < 1$ and $x := (x_1, x_2) \in \Omega$, we look for the function u satisfying

$$(5.1) \quad \begin{cases} {}^C_0 D^\nu_t u(x,t) - \Delta u(x,t) = f(x,t), & (x,t) \in \Omega \times (0,T], \\ u(x,0) = 0, & x \in \Omega, \\ u(x,t)\big|_{\partial\Omega} = 0, & t \in (0,T). \end{cases}$$

Here we choose the source term

$$(5.2) \quad f(x,t) = t^{0.3}(1 - |2x_1 - 1|)(1 - |2x_2 - 1|).$$

In our computation, the domain $\Omega = (0,1)^2$ is first divided into M^2 small equal squares, and we obtain a symmetric triangulation by connecting the diagonal of each small square. To verify the temporal error, we fixed $M = 100$, $\beta = 5$ and changed the number of basis functions of the spectral method in the time direction. Since the closed form of the exact solution to problem (5.1) is unavailable, we compute a reference solution $u_h \approx u_{hN_{ref}}$, with $N_{ref} = 70$.

In this case, the source term f satisfies the smoothness requirement in Theorems 4.5 and 4.8,

$$(5.3) \quad \partial^j_t(t^j f) \in L^2_{\chi^k_T}(\Lambda; H^1_0(\Omega)) \quad \forall 0 \leq j \leq k \text{ and } k = 0, 1, \ldots, m,$$

with an arbitrary positive integer m. Therefore, all the theoretical results hold valid and we expect an exponential convergence in the time direction. The numerical results are presented in Figure 2, where the temporal error E_L in L^2 space and error E_H in space-time energy space are defined by

$$(5.4) \quad E_L = \frac{\|u_h - u_{hN}\|_{L^2(\Lambda; L^2(\Omega))}}{\|u_h\|_{L^2(\Lambda; L^2(\Omega))}} \quad \text{and} \quad E_H = \frac{\|u_h - u_{hN}\|_{H^{\frac{\nu}{2},1}(\mathcal{O})}}{\|u_h\|_{H^{\frac{\nu}{2},1}(\mathcal{O})}},$$

respectively. In Figure 2, we draw the error curves against N for distinct parameters ν and final time T. All the experiments show that the proposed spectral-Galerkin method is highly efficient for subdiffusion problems, and the numerical solutions u_{hN} exponentially converge to u_h.

Next, we test the problem (5.1) with another source term,

$$(5.5) \quad f(x,t) = (1 + t^{0.5})x_1(1 - x_1)x_2(1 - x_2),$$

and compare the spectral-Galerkin method with some high-order BDF schemes developed in [27]. Note that the source is nonsmooth in the time direction, and hence the BDF schemes fail to achieve the desired high accuracy. In particular, it can be verified that

$$f \in W^{\frac{3}{2}-\epsilon,1}(0, T/2; L^2(\Omega)) \cap W^{m,\infty}(T/2, T; L^2(\Omega))$$

for any small $\epsilon > 0$ and positive integer $m > 0$. The proof of [27, Theorem 2.2] indicates a convergence rate $O(\tau^{\frac{3}{2}-\epsilon})$ for this example, where τ denotes the step size in time. This prediction is consistent with the numerical results plotted in Figure 3 (right), where we plot the $L^2(\Omega)$-norm of the numerical error at $T = 1$. On the other hand, the source term still satisfies the smoothness requirement (5.3). Therefore, we can observe the high accuracy of the spectral method in Figure 3 (left). Those experiments indicate that the spectral-Galerkin method (4.19) performs much better than the time-stepping approach in this special case.
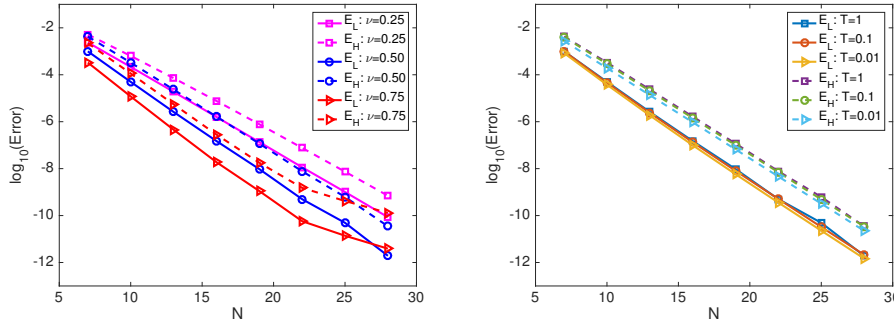
FIG. 2. *Example* (a) *with the source term* (5.2). *Left: plot of* E_L *and* E_H *with* $T = 1$ *and fractional orders* $\nu = 0.25, 0.5, 0.75$. *Right: plot of* E_L *and* E_H *with* $\nu = 0.5$ *and terminal times* $T = 0.01, 0.1, 1$.
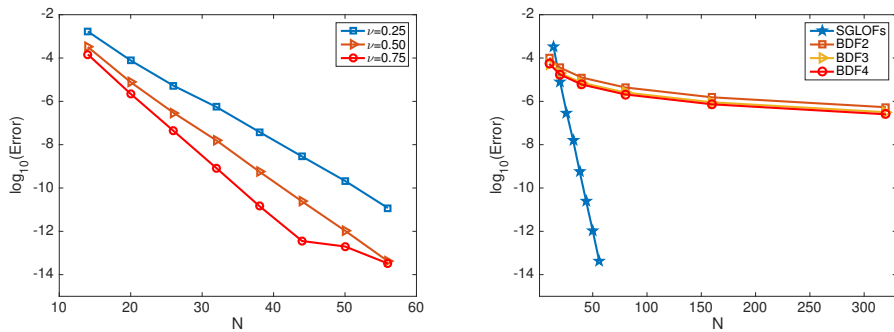

FIG. 3. *Example* (a) *with the source term* (5.5). *Left: plot of* E_L *with* $T = 1$ *and fractional orders* $\nu = 0.25, 0.5, 0.75$. *Right: plot of the* $L^2(\Omega)$-*norm of the error at* $T = 1$ *with* $\nu = 0.5$ *for spectral-Galerkin method* (4.19) *and the* k*th-order BDF method proposed in* [27].

Example (b). Subdiffusion problems with time-dependent coefficients.
We consider the following subdiffusion problems with time-dependent coefficients:

$$(5.6) \quad \begin{cases} {}_0\mathrm{D}_t^\nu u(x,t) - \nabla \cdot (a(x,t)\nabla u(x,t)) = f(x,t), & x \in \Omega, \ t \in \Lambda := (0,T), \\ u(x,t) = 0, & (x,t) \in \partial\Omega \times (0,T], \\ u(x,0) = 0, & x \in \Omega. \end{cases}$$

Here we assume that the diffusion coefficient $a(x,t) : \Omega \times (0,T) \to \mathbb{R}^{d \times d}$ has the following regularity for some real number $\lambda \geq 1$ and for any positive integer m:

$$(5.7)$$
$$\lambda^{-1}|\xi|^2 \leq a(x,t)\xi \cdot \xi \leq \lambda|\xi|^2 \qquad \forall \xi \in \mathbb{R}^d, \ \forall (x,t) \in \Omega \times (0,T],$$
$$(5.8)$$
$$\left|\tfrac{\partial}{\partial t}a(x,t)\right| + |\nabla_x a(x,t)| + \left|\nabla_x \tfrac{\partial}{\partial t}a(x,t)\right| \leq c \quad \forall (x,t) \in \Omega \times (0,T],$$
$$(5.9)$$
$$\left|\nabla_x \tfrac{\partial^j}{\partial t^j}a(x,t)\right| + \left|\nabla_x \tfrac{\partial^{j+1}}{\partial t^{j+1}}a(x,t)\right| \leq c \qquad \forall (x,t) \in \Omega \times (0,T], \ j = 1, \ldots, m.$$

For standard parabolic problems with time-dependent coefficients, there are a few relevant works. Unfortunately, the fractional derivative does not satisfy the well-known Leibnitz rule, and hence some traditional techniques working for the heat equation

cannot be directly applied. In [46], Mustapha analyzed the spatially semidiscrete Galerkin FEM approximation of the subdiffusion problem involving time-dependent coefficients, but without the source term, by using a novel energy argument. A perturbation argument was developed in [29] to derive regularity results and analyze the spatially semidiscrete Galerkin scheme, as well as some first-order time stepping schemes. In particular, it has been proved in [29, Theorem 2.1] that under conditions (5.7)–(5.9), with $u_0 = 0$ and $f \in L^p(0, T; L^2(\Omega))$, $1/\alpha < p < \infty$, problem (2.6) has a unique solution

$$u \in C([0, T]; L^2(\Omega)) \cap L^p(0, T; \dot{H}^2(\Omega)) \quad \text{such that} \quad {}_0\mathrm{D}_t^\nu u \in L^p(0, T; L^2(\Omega)).$$

Very recently, a second-order time stepping scheme, based on convolution quadrature generated by the second-order BDF scheme and an initial correction technique, was developed and analyzed in [26]. To the best of our knowledge, there is no other high-order numerical scheme for such models with rigorous analysis in the literature. The main difficulty is caused by the initial singularity of the solution, which will cause trouble in the estimation of the perturbation term. However, under the assumptions (5.7)–(5.9), it has been proved in [26, Theorem 3.2] that the solution u satisfies the regularity results for all $t \in (0, T]$ and $k \in \mathbb{N}$:

$$(5.10) \qquad \left\| \partial_t^k (t^k u(t)) \right\|_{\dot{H}^3(\Omega)} \leq c \sum_{j=0}^k t^j \| f^{(j)}(0) \|_{\dot{H}^1(\Omega)} + ct^k \int_0^t \| f^{(k)}(s) \|_{\dot{H}^1(\Omega)} \mathrm{d}s.$$

Therefore, using this estimate, we have the following result.

THEOREM 5.1. *Assuming that* $f \in W^{m+1,1}(\Lambda; \dot{H}^1(\Omega))$, *the solution u of the subdiffusion problem* (5.6) *satisfies*

$$\partial_{\gamma,t}^k ({}_0\mathrm{D}_t^{\frac{\nu}{2}} u) \in L^2_{\chi_T^k}(\Lambda; H_0^1(\Omega)) \quad for \ \ k = 0, 1, \ldots, m,$$

where $\partial_{\gamma,t} = t\partial_t - \gamma$, *with* $\gamma > 0$.

The proof of Theorem 5.1 can be found in Appendix C. This result indicates that ${}_0\mathrm{D}_t^{\frac{\nu}{2}} u(x, t)$ belongs to the nonuniformly weighted Sobolev space $A_{\frac{\beta}{2},T}^m(\Lambda; H_0^1(\Omega))$, provided that the source term is smooth enough in the time direction. This regularity result motivates us to develop a spectral-Galerkin method using the LOFs. In fact, it is possible to prove such a regularity result as above in the case where f satisfies the smoothness requirement (5.3). But the proof requires some technical arguments and is out of the scope of the current paper.

Let $X_N^t(\Lambda)$ and $X_h^x(\Omega)$ be finite-dimensional spaces defined in (4.4) and (4.12), respectively. Then our fully discrete scheme for (5.6) reads as follows: find $u_{hN} \in X_{hN} := X_N^t \otimes X_h^x$ such that

$$(5.11) \quad \int_0^T \left({}_0\mathrm{D}_t^{\frac{\nu}{2}} u_{hN} \, , {}_t\mathrm{D}_T^{\frac{\nu}{2}} v \right)_\Omega + \left(a(t)\nabla u_{hN}, \nabla v \right) \mathrm{d}t = \int_0^T (f, v)_\Omega \, \mathrm{d}t \quad \forall v \in X_N^t \otimes X_h^x.$$

In the first experiment, we let $a(x, t) := 2 + \cos(t)$, $\Omega = (0, 1)^2$, $T = 1$, and we test

$$(5.12) \qquad\qquad f(x, t) = \cos(t) x_1(1 - x_1) x_2(1 - x_2),$$

which is smooth in the time direction. Therefore, by Theorem 5.1 and the approximation property in Lemma 3.2, we expect that the numerical solution u_{hN} converges
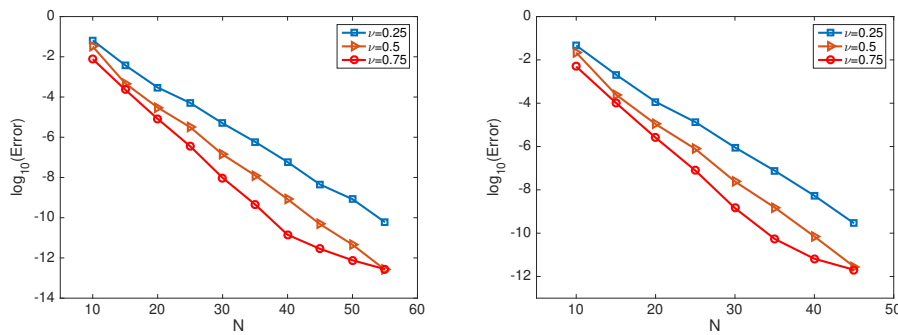
FIG. 4. *Example* (b). *Left: plot of E_L with $T = 1$, with the smooth-in-time source term* (5.12) *and fractional orders $\nu = 0.25, 0.5, 0.75$. Right: plot of E_L with $T = 1$, with the nonsmooth-in-time source term* (5.12) *and fractional orders $\nu = 0.25, 0.5, 0.75$.*

to u_h exponentially. This estimate is fully supported by the error curves (against N) plotted in Figure 4 (left).

Further, we test the numerical results in the case of nonsmooth (in time) source term

$$(5.13) \qquad f(x,t) = (1 + t^{0.1})x_1(1 - x_1)x_2(1 - x_2).$$

Although it does not satisfy the smoothness condition in Theorem 5.1, we still observe the exponential convergence (see, e.g., Figure 4 (right)). The theoretical confirmation awaits studies in the future. The numerical results verify the high efficiency of the spectral-Galerkin method for solving the subdiffusion problem with time-dependent coefficients.

Example (c). Time-fractional Allen–Cahn equations. Finally, we consider the following one-dimensional time-fractional Allen–Cahn problem:

$$(5.14) \qquad \begin{cases} {}_0^C\mathrm{D}_t^\nu u - \epsilon^2 \Delta u = u - u^3, & x \in \Omega := (-1, 1), \ t > 0, \\ u(-1, t) = u(1, t) = 0, & t \geq 0, \\ u(x, 0) = u_0(x), & x \in \Omega, \end{cases}$$

where ε is a small parameter which describes the interfacial width.

The first rigorous studies of the semilinear subdiffusion problem were given in [28], where Jin, Li, and Zhou proposed a general framework for mathematical and numerical analysis of the semilinear subdiffusion equation with a globally Lipschitz continuous potential $f(u)$. A time-stepping scheme based on a backward Euler convolution quadrature scheme was studied, and a convergence rate of order $O(\tau^\alpha)$ was proved, where τ denotes the step size in time. Then the analysis was extended to the time-fractional Allen–Cahn equation [13], where Du, Yang, and Zhou developed and analyzed several αth-order accurate time-stepping schemes satisfying a weighted energy dissipation law. See also [2] for the argument in the case of nonsmooth initial data. As far as we know, high-order time-stepping schemes by using convolution quadrature or a collocation method for the nonlinear problem (5.14) are still missing in the literature.

In order to develop a spectral-Galerkin scheme for solving the time-fractional Allen–Cahn equation (5.14), we define an auxiliary function $w(x, t) = u(x, t) - u_0(x)$

and note that the function $w(x,t)$ satisfies the following initial boundary value problem:

$$\begin{cases} F(w) := {}^C_0 \mathrm{D}^\nu_t w - \varepsilon^2 \Delta w + (w + u_0)^3 - w - (\varepsilon^2 \Delta u_0 + u_0) = 0, & x \in \Omega, \ t > 0, \\ w(-1,t) = w(1,t) = 0, & t \geq 0, \\ w(x,0) = 0, & x \in \bar{\Omega}. \end{cases}$$

Using the Newton iterative method [55], we are led to solve, at each iteration,

$$\begin{cases} {}^C_0 \mathrm{D}^\nu_t E_k - \varepsilon^2 \Delta E_k + (3(w_k + u_0)^2 - 1)E_k = -F(w_k), & x \in \Omega, \ t > 0, \\ E_k(-1,t) = E_k(1,t) = 0, & t \geq 0, \\ E_k(x,0) = 0, & x \in \Omega, \\ w_{k+1} = E_k + w_k, & x \in \Omega, \ t \geq 0. \end{cases}$$

In the computation, we choose the initial guess $w_0 = 0$ and derive the approximation $w_{k+1} = w_k + E_k$ by the above iteration process. For each iteration step, we apply the fully discrete method (4.19).

In our computation, we test the time-fractional Allen–Cahn equation (5.14) with $\varepsilon = 0.05$, $h = 0.01$, $\beta = 7$, and smooth initial distribution $u_0(x) = \sin \pi x$. The profile of the numerical solution at $T = 10$ is plotted in Figure 5 (left). Furthermore, in order to verify the high efficiency of the spectral-Galerkin method in time, we plot the error curve in Figure 5 (right). The exponential decay of the error shows again that our new method is very efficient for solving the semilinear time-fractional problem (5.14).
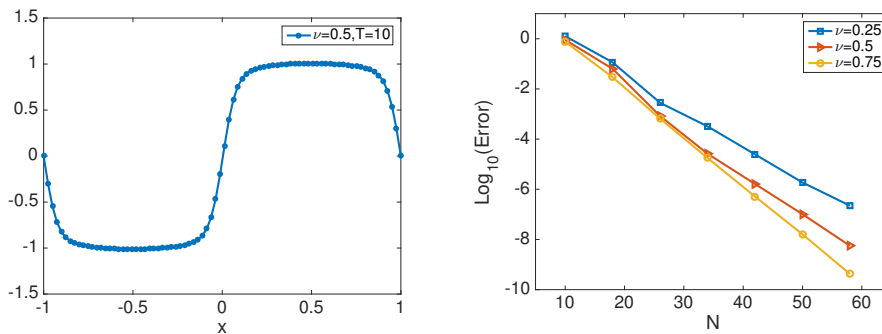

FIG. 5. *Example* (c). *Left: profile of numerical solutions at $T = 10$. Right: plot of E_L with $T = 10$ and $\nu = 0.25, 0.5, 0.75$.*

6. Conclusion. In this paper, we developed a spectral-Galerkin method (in the time direction) for solving the subdiffusion equations which involve a time-fractional derivative with order $\nu \in (0,1)$. The log orthogonal functions (LOFs), which were constructed by applying a log mapping to the Laguerre functions, are used as the basis functions. We established the regularity results in some nonuniform weighted Sobolev spaces. This together with the approximation properties of the LOFs leads to the spectral convergence of the numerical schemes. We believe that this is the first such result with spectral accuracy in time for weakly singular solutions of subdiffusion problem (1.1).

We also developed fully discrete space-time schemes with the spectral-Galerkin method in time and the Galerkin finite element method in space. Compared with the traditional time-stepping schemes, the proposed spectral-Galerkin method in time

could achieve high accuracy even if both the solution and the source term have singularities at initial time, and hence it is very efficient for solving the subdiffusion problem. Numerical results fully support the efficiency and accuracy of the proposed spectral-Galerkin methods.

Furthermore, we have applied the proposed method to linear subdiffusion equations with time-dependent diffusion coefficients as well as nonlinear subdiffusion equations, for which high-order time-stepping schemes are rarely studied in the literature. Our numerical results indicate that the proposed approach is very efficient and achieves accuracy similar to that for the linear subdiffusion equations with time-independent coefficients.

Appendix A. The detail for computing $\mathbf{M}^t$ and $\mathbf{S}^t$. In this section, we shall present the way to compute the mass matrix $\mathbf{M}^t$ and stiffness matrix $\mathbf{S}^t$.

In fact, by using the Gauss-GLOFs quadrature (3.1) and relation

$$
m_{qn}^t = \left(\widehat{\mathcal{S}}_n^\nu, \widehat{\mathcal{S}}_q^\nu \right) = \int_0^T \left(\frac{t}{T} \right)^{\frac{\nu}{2}} \mathcal{S}_n \left(\frac{t}{T} \right) \left(\frac{t}{T} \right)^{\frac{\nu}{2}} \mathcal{S}_q \left(\frac{t}{T} \right) \mathrm{d}t = T \int_0^1 \tau^\nu \mathcal{S}_n(\tau) \mathcal{S}_q(\tau) \, \mathrm{d}\tau,
$$

we can compute $\mathbf{M}^t$ with high accuracy.

The evaluation of $\mathbf{S}^t$, involving the fractional derivative, is more technical. The following relation eases the complexity:

$$
s_{qn}^t = \left({}_0\mathrm{D}_t^{\frac{\nu}{2}} \widehat{\mathcal{S}}_n^\nu, {}_t\mathrm{D}_1^{\frac{\nu}{2}} \widehat{\mathcal{S}}_q^\nu \right) = \left({}_0\mathrm{D}_t^\nu \widehat{\mathcal{S}}_n, \widehat{\mathcal{S}}_q \right) = \int_0^T {}_0\mathrm{D}_t^\nu \left\{ \left(\frac{t}{T} \right)^{\frac{\nu}{2}} \mathcal{S}_n \left(\frac{t}{T} \right) \right\} \left(\frac{t}{T} \right)^{\frac{\nu}{2}} \mathcal{S}_q \left(\frac{t}{T} \right) \mathrm{d}t
$$

$$
= T^{1-\nu} \int_0^1 {}_0^C\mathrm{D}_\tau^\nu \left\{ \tau^{\frac{\nu}{2}} \mathcal{S}_n(\tau) \right\} \tau^{\frac{\nu}{2}} \mathcal{S}_q(\tau) \, \mathrm{d}\tau,
$$

where the last equality holds via $\widehat{\mathcal{S}}_n^\nu(0) = 0$ and the relation (see [11, equation (2.9)]) below:

$$
{}_0\mathrm{D}_t^\nu h \left(\frac{t}{T} \right) = T^{-\nu} {}_0\mathrm{D}_\tau^\nu h(\tau), \quad \tau = \frac{t}{T}.
$$

Next, denote $f(t) = t^{\frac{\nu}{2}} \mathcal{S}_n(t)$ and $g(t) = t^{\frac{\nu}{2}} \mathcal{S}_m(t)$; then the remaining work is to compute

$$
\int_0^1 \frac{1}{\Gamma(1-\nu)} \int_0^t \frac{f'(s)}{(t-s)^\nu} \, \mathrm{d}s \, g(t) \mathrm{d}t \overset{s=t\tau}{=} \frac{1}{\Gamma(1-\nu)} \int_0^1 \int_0^1 \frac{f'(t\tau)}{(1-\tau)^\nu} \, \mathrm{d}\tau \, g(t) t^{1-\nu} \mathrm{d}t.
$$

The integrand $f(t\tau) \, g(t) t^{1-\nu} (1-\tau)^{-\nu}$ has the low regularity near both $t \to 0$ and $t \to 1$. In order to compute integral $\int_0^1 {}_0^C\mathrm{D}_t^\nu f(t) \, g(t) \mathrm{d}t$ with high accuracy, we use the identity

$$
\int_0^1 \frac{f'(t\tau)}{(1-\tau)^{-\nu}} \, \mathrm{d}\tau = \int_0^{\frac{1}{2}} f'(t\tau)(1-\tau)^{-\nu} \, \mathrm{d}\tau + \int_{\frac{1}{2}}^1 f'(t\tau)(1-\tau)^{-\nu} \, \mathrm{d}\tau
$$

$$
= \frac{1}{2} \int_0^1 f' \left(\frac{t\tau}{2} \right) \left(1 - \frac{\tau}{2} \right)^{-\nu} \mathrm{d}\tau + \frac{1}{4^{1-\nu}} \int_{-1}^1 f' \left(\frac{t(x+3)}{4} \right) (1-x)^{-\nu} \, \mathrm{d}x,
$$

to derive its high accuracy numerical approximation,

$$
\int_0^1 {}_0^C\mathrm{D}_t^\nu f(t) \, g(t) \mathrm{d}t \approx \frac{1}{2\Gamma(1-\nu)} \sum_{i=0}^{N_L} \sum_{j=0}^{N_L} f' \left(\frac{t_i \, t_j}{2} \right) \left(1 - \frac{t_j}{2} \right)^{-\nu} g(t_i) t_i^{1-\nu} \, \chi_i \chi_j
$$

$$
+ \frac{1}{4^{1-\nu}\Gamma(1-\nu)} \sum_{i=0}^{N_L} \sum_{j=0}^{N_J} f' \left(\frac{t_i(\xi_j+3)}{4} \right) g(t_i) t_i^{1-\nu} \, \chi_i \eta_j,
$$

where N_L and N_J are the node numbers usually greater than the degree of polynomials/functions, and the corresponding Gauss nodes and weights $\{t_i, \chi_i\}_{i=0}^{N_I}$ and $\{\xi_i, \eta_i\}_{i=0}^{N_I}$ are the Gauss-GLOFs nodes with suitable β and the classical Gauss–Jacobi nodes with weight function $\omega^{-\nu,0} = (1-x)^{-\nu}$, respectively. $\qquad\qquad\square$

Appendix B. Proof of Lemma 4.7. Repeating the argument in (4.8)–(4.11), we have the following expression for any $v \in X_h^x$:

$$
{}_0\mathrm{D}_t^{\frac{\nu}{2}} u_h = \int_0^t \bar{E}_h(t-s) P_h f(s)\, ds, \quad \text{where} \quad \bar{E}_h(t)v = \sum_{n=1}^{\infty} t^{\frac{\nu}{2}-1} E_{\nu,\frac{\nu}{2}}(-\lambda_n^h t^\nu)(v, \varphi_n^h)_\Omega.
$$

Then similar to Lemma 4.4, there holds the smoothing property

$$
\|\partial_t^k (t^k \bar{E}_h(t)) v\|_{L^2(\Omega)} \le c t^{\frac{\nu}{2}-1} \|v\|_{L^2(\Omega)} \quad \forall v \in X_h^x \quad \text{and} \quad k = 0,1,2,\ldots.
$$

Next, by the observation

$$
\lim_{t \to 0} t^{k+1} \partial_t^k f(t) = 0 \quad \text{and} \quad \lim_{t \to 0} \|t^{k+1} \partial_t^k \bar{E}_h(t) v\|_{L^2(\Omega)} = 0 \quad \forall v \in L^2(\Omega)
$$

and simple calculation, we derive that

$$
\begin{aligned}
\partial_t^k \big(t^k [{}_0\mathrm{D}_t^{\frac{\nu}{2}}(-L_h)^{\frac{1}{2}} u_h]\big)(t) &= \partial_t^k \left(t^k \int_0^t \bar{E}_h(t-\tau)(-L_h)^{\frac{1}{2}} P_h f(\tau)\, d\tau \right) \\
&= \sum_{j=0}^k \binom{k}{j} \partial_t^k \left(\int_0^t (t-\tau)^{k-j} \bar{E}_h(t-\tau)\, \tau^j (-L_h)^{\frac{1}{2}} P_h f(\tau) d\tau \right) \\
&= \sum_{j=0}^k \binom{k}{j} \int_0^t \left(\partial_t^{k-j} [(t-\tau)^{k-j} \bar{E}_h(t-\tau)] \right) \left(\partial_\tau^j [\tau^j (-L_h)^{\frac{1}{2}} P_h f(\tau)] \right) d\tau,
\end{aligned}
$$

where we apply the estimate that

$$
c_1 \|v\|_{\dot{H}^1(\Omega)} \le \|(-L_h)^{\frac{1}{2}} v\|_{L^2(\Omega)} \le c_2 \|v\|_{\dot{H}^1(\Omega)} \quad \forall v \in X_h^x.
$$

Appealing to Lemma 4.4, we have the estimate that

$$
\begin{aligned}
\|\partial_t^k \big(t^k [{}_0\mathrm{D}_t^{\frac{\nu}{2}} u_h]\big)(t)\|_{\dot{H}^1(\Omega)} &= \|\partial_t^k \big(t^k [{}_0\mathrm{D}_t^{\frac{\nu}{2}}(-L_h)^{\frac{1}{2}} u_h]\big)(t)\|_{L^2(\Omega)} \\
&\le c \sum_{j=0}^k \int_0^t (t-\tau)^{\frac{\nu}{2}-1} \|\partial_\tau^j [\tau^j P_h f(\tau)]\|_{\dot{H}^1(\Omega)}\, d\tau =: c \sum_{j=0}^k K_j(t).
\end{aligned}
$$

Then Young's convolution inequality and the stability of $L^2(\Omega)$ projection P_h on $\dot{H}^1(\Omega)$ imply that

$$
\begin{aligned}
\int_0^T |K_j(t)|^2 |\log(t/T)|^k\, dt &= \int_0^T \left| \int_0^t (t-\tau)^{\frac{\nu}{2}-1} \|P_h \partial_\tau^j [\tau^j f(\tau)]\|_{\dot{H}^1(\Omega)}\, d\tau \right|^2 |\log(t/T)|^k\, dt \\
&\le c \int_0^T \left| \int_0^t (t-\tau)^{\frac{\nu}{2}-1} \left(\|\partial_\tau^j [\tau^j f(\tau)]\|_{\dot{H}^1(\Omega)} |\log(\tau/T)|^{\frac{k}{2}} \right) d\tau \right|^2 dt \\
&\le c \left(\int_0^T t^{\frac{\nu}{2}-1}\, dt \right)^2 \int_0^T \|\partial_\tau^j [\tau^j f(\tau)]\|_{\dot{H}^1(\Omega)}^2 |\log(\tau/T)|^k\, dt \\
&\le c \int_0^T \|\partial_\tau^j [\tau^j f(\tau)]\|_{\dot{H}^1(\Omega)}^2 |\log(\tau/T)|^k\, dt \le c.
\end{aligned}
$$

Therefore, $\partial_t^k\big(t^k[_0\mathrm{D}_t^{\frac{\nu}{2}}u]\big) \in L^2_{\chi_T^k}(\Lambda; H_0^1(\Omega))$ for $k = 0, 1, \ldots, m$, and so does $\partial_{\gamma,t}^k[_0\mathrm{D}_t^{\frac{\nu}{2}}u]$. This completes the proof of this lemma. $\qquad\square$

Appendix C. Proof of Theorem 5.1. It suffices to show that $\partial_t^k(t^k{}_0\mathrm{D}_t^{\frac{\nu}{2}}u) \in L^2_{\chi_T^k}(\Lambda; H_0^1(\Omega))$ for all $k = 0, 1, \ldots, m$. Appealing to the subdiffusion equation (5.6), we have

$$_0\mathrm{D}_t^{\frac{\nu}{2}}u(t) = \int_0^t \frac{(t-\tau)^{\nu/2-1}}{\Gamma(\nu/2)} L(\tau)u(\tau)\, d\tau + \int_0^t \frac{(t-\tau)^{\nu/2-1}}{\Gamma(\nu/2)} f(s)\, ds.$$

Using the a priori estimate (5.10), we derive that for all $k = 0, 1, \ldots, m-1$

$$\lim_{t\to 0} \partial_t^k(t^{k+1}u(t)) = 0 \quad\text{and}\quad \lim_{t\to 0} \partial_t^k(t^{k+1}f(t)) = 0,$$

and hence

$$\partial_t^k(t^k{}_0\mathrm{D}_t^{\frac{\nu}{2}}u(t)) = \frac{1}{\Gamma(\nu/2)} \sum_{j=0}^k \binom{k}{j} \int_0^t \partial_t^j(t-\tau)^{\nu/2+j-1}\partial_\tau^{k-j}\big[\tau^{(k-j)}(L(\tau)u(\tau) + f(\tau))\big]\, d\tau.$$

Then taking the $\dot{H}^1(\Omega)$ norm, we obtain

$$\|\partial_t^k(t^k{}_0\mathrm{D}_t^{\frac{\nu}{2}}u(t))\|_{\dot{H}^1(\Omega)} \le c \sum_{j=0}^k \int_0^t (t-\tau)^{\nu/2-1}\big[\|\partial_\tau^j(\tau^j u(\tau))\|_{\dot{H}^3(\Omega)} + \|\partial_\tau^j(\tau^j f(\tau))\|_{\dot{H}^1(\Omega)}\big]\, d\tau \le c.$$

This immediately implies that $\partial_t^k(t^k{}_0\mathrm{D}_t^{\frac{\nu}{2}}u(t)) \in L^2_{\chi_T^k}(\Lambda; H_0^1(\Omega))$.

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