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RATIONAL SPECTRAL METHODS FOR PDEs INVOLVING FRACTIONAL LAPLACIAN IN UNBOUNDED DOMAINS*

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Abstract. Many PDEs involving fractional Laplacian are naturally set in unbounded domains with underlying solutions decaying slowly and subject to certain power law. Their numerical solutions are underexplored. This paper aims at developing accurate spectral methods using rational basis (or modified mapped Gegenbauer functions) for such models in unbounded domains. The main building block of the spectral algorithms is the explicit representations for the Fourier transform and fractional Laplacian of the rational basis, derived from some useful integral identities related to modified Bessel functions. With these at our disposal, we can construct rational spectral-Galerkin and direct collocation schemes by precomputing the associated fractional differentiation matrices. We obtain optimal error estimates of rational spectral approximation in the fractional Sobolev spaces and analyze the optimal convergence of the proposed Galerkin scheme. We also provide ample numerical results to show that the rational method outperforms the Hermite function approach.

Key words. fractional Laplacian, Gegenbauer polynomials, modified rational functions, unbounded domains, Fourier transforms, spectral methods

AMS subject classifications. 65N35, 65M70, 41A05, 41A25

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1. Introduction.

Diffusion is a ubiquitous physical process, typically modeled by partial differential equations (PDEs) with the usual Laplacian operators. Although they can describe the anisotropy of diffusion, many systems in science, economics, and engineering exhibit anomalous diffusion, which can be more accurately and realistically modeled by PDEs with fractional Laplacian operators [4, 5, 12]. In the past decade, tremendous research attention has been paid to the analysis and numerical studies of fractional PDEs. The finite difference method and the finite element method are two widely studied methods in this direction (see, e.g., [17, 18, 19, 9, 40, 3, 42, 36, 43] and references therein). Most efforts are devoted to dealing with the nonlocal nature or singularities of the fractional operators. Another powerful approach is the spectral method, which is more suitable for the nonlocal feature

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of the fractional operators (see, e.g., [45, 10, 27, 20, 24, 34, 35, 44, 37, 48, 46, 47]). However, most of these works are for fractional problems in bounded domains. In particular, we refer to Bonito et al. [6] for an up-to-date review of the various numerical methods for fractional diffusion based on different formulations of the fractional Laplacian.

It is known that many physically motivated fractional diffusive problems are naturally set in unbounded domains, but their investigation is still underexplored. For usual PDEs in unbounded domains, several approaches have been widely used in practice (see, e.g., [8, 32] and the original references cited therein). The first is direct domain truncation, which works well for problems with rapidly decaying solutions but is not feasible for fractional problems as the underlying solutions usually decay slowly (and subject to certain power laws at infinity). On the other hand, the naive truncation introduces nonphysical singularities at the interface where the unbounded domain is terminated. The second is to design a suitable transparent boundary condition or artificial sponge layer, but this appears highly nontrivial for the fractional Laplacian. The third is the use of orthogonal functions in unbounded domains, which has been successfully applied to many usual PDEs (see, e.g., [38, 8, 13, 26, 32, 31]). Very recently, spectral methods for fractional PDEs on the half line have been proposed by [21, 24]—using the generalized Laguerre functions as basis functions—extending the idea of [45]. A two-domain spectral approximation by Laguerre functions is developed in [11] for tempered fractional PDEs on the whole line. Mao and Shen [28] proposed both spectral-Galerkin and collocation methods using Hermite functions for fractional PDEs in unbounded domains. However, the collocation method therein relies on an equivalent formulation in frequency space by the Fourier transforms and performs collocation methods to the equivalent formulation that involve forward/backward Hermite transforms. Tang, Yuan, and Zhou [39] developed *direct* Hermite collocation methods with explicit formulations for the differentiation matrices, which is therefore more robust for nonlinear problems. Last, spectral approximation using nonclassical orthogonal functions in unbounded domains—image of classical Jacobi polynomials through a suitable mapping—has proven to be more viable for usual PDEs with solutions decaying algebraically (see, e.g., [7, 8, 15, 16, 30]), compared with approximation by Hermite/Laguerre functions. As such, the rational basis (or mapped Jacobi functions) should be more desirable for PDEs with fractional Laplacian, due to the slow decaying solution with long tails subject to certain power law. However, to the best of our knowledge, there is essentially no work available along this line. Moreover, the extension of the mapping technique to the fractional setting is far from trivial, as we elaborate on below.

In this paper, we intend to fill in this gap and design rational spectral methods for a class of PDEs with fractional Laplacian in $\mathbb{R}^d$. To fix the idea, we consider the model equation

$$\begin{cases} (-\Delta)^{\alpha/2}u(x) + \rho u(x) = f(x), & x \in \mathbb{R}^d, \\ u(x) \to 0, & |x| \to \infty, \end{cases} \tag{1.1}$$

for $\rho > 0$ and $\alpha \in (0, 2)$, where the fractional Laplace operator is defined as in [22]:

$$(-\Delta)^{\alpha/2}u(x) := C_{d,\alpha}\text{p.v.}\int_{\mathbb{R}^d} \frac{u(x) - u(y)}{|x - y|^{d+\alpha}}dy \quad \text{with} \quad C_{d,\alpha} := \frac{\alpha 2^{\alpha-1}\Gamma\Big(\dfrac{\alpha+d}{2}\Big)}{\pi^{d/2}\Gamma\Big(\dfrac{2-\alpha}{2}\Big)}. \tag{1.2}$$

Here, p.v. stands for the Cauchy principal value, and $C_{d,\alpha}$ is a normalization constant. Equivalently, the fractional Laplacian can be defined as a pseudodifferential operator via the Fourier transform:

$$(-\Delta)^{\alpha/2}u(x) := \mathscr{F}^{-1}\big[|\xi|^{\alpha}\mathscr{F}[u](\xi)\big](x). \tag{1.3}$$

For spectral-Galerkin and collocation methods, a critical issue is how to accurately evaluate the fractional Laplacian performing on the basis functions. For example, the key to the Hermite spectral method in [28] is the use of the attractive property that the Hermite functions are the eigenfunctions of the Fourier transform, so the algorithm is largely implemented in the frequency ξ-space. In contrast, some analytically perspicuous formulas of $(-\Delta)^{\alpha/2}$ on the Hermite functions were derived in [39], which led to the construction of efficient collocation algorithms in the physical x-space. In the spirit of [39], we search for the analytic formulas for computing the fractional Laplacian of the rational basis functions—the modified mapped Gegenbauer functions (MMGFs), orthogonal with respect to a uniform weight. Although the formulas (see Theorem 3.4) are not as compact as those for the Hermite functions, we can accurately compute the fractional Laplacian of the rational basis up to the degree $\sim 10^3$ by using, e.g., Maple or Mathematica. Moreover, with these analytic tools at our disposal, we are able to study their asymptotic behaviors and dependence of the parameters so that the basis can be tailored to the decay rate of the underlying solution. We propose and analyze a spectral-Galerkin scheme and obtain optimal estimates (see Theorem 5.1). We also implement a direct collocation scheme based on the associated fractional differentiation matrices with the aid of the aforementioned explicit formulas. However, its error analysis appears very challenging and largely open. This is mostly for the reason that the fractional Laplacian takes the rational basis to a class of functions of completely different nature, as opposite to the usual Laplacian. In the multidimensional case, we implement the collocation schemes in the frequency space (cf. [28]), which relies on the approximability of spectral expansions to $\mathscr{F}[f](\xi)/(|\xi|^{\alpha}+\rho)$ for given source term f. We show that the rational approach outperforms the Hermite method (cf. [28]) in two dimensions. In fact, it is common that the Fourier transform of a function decays much slower than the function itself, so the rational basis is more desirable in this context.

The rest of the paper is organized as follows. In section 2, we collect some useful properties of the Bessel functions and Gegenbauer polynomials. In section 3, we present the main formulas for computing the fractional Laplacian of the modified rational functions and study the asymptotic properties. In section 4, we derive optimal error estimates of the approximation by the modified rational functions in fractional Sobolev spaces. We propose and analyze spectral-Galerkin methods using modified rational basis functions in section 5. Then we implement the collocation methods in both one dimension and multiple dimensions in section 6. The final section is for some concluding remarks.

2. Preliminaries.

In this section, we make necessary preparations for the algorithm development and analysis in the forthcoming sections. More precisely, we review some relevant properties of hypergeometric functions, Gegenbauer polynomials, Bessel functions, and their interwoven relations.

2.1. Bessel functions.

Recall that the Bessel function of the first kind of real order μ has the series expansion (cf. [29]):

$$J_{\mu}(x) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!\,\Gamma(m+\mu+1)}\Big(\frac{x}{2}\Big)^{2m+\mu}. \tag{2.1}$$

The modified Bessel functions of the first and second kinds are defined by

$$I_\mu(x) = \mathrm{i}^{-\mu} J_\mu(\mathrm{i}x), \quad K_\mu(x) = \frac{\pi}{2}\frac{I_{-\mu}(x) - I_\mu(x)}{\sin(\mu\pi)}, \tag{2.2}$$

respectively, where $\mathrm{i} = \sqrt{-1}$ is the complex unit. For the modified Bessel functions of the second kind $K_\mu(x)$, we have the following important integral identities (see [14, p. 738]): for $-\lambda \pm \mu < 1$ and $a, b > 0$,

$$\begin{aligned}\int_0^\infty x^\lambda K_\mu(ax)\cos(bx)dx = {}& 2^{\lambda-1}a^{-\lambda-1}\Gamma\Big(\frac{\mu+\lambda+1}{2}\Big)\Gamma\Big(\frac{1+\lambda-\mu}{2}\Big)\\ &\times {}_2F_1\Big(\frac{\mu+\lambda+1}{2}, \frac{1+\lambda-\mu}{2}; \frac{1}{2}; -\frac{b^2}{a^2}\Big),\end{aligned} \tag{2.3}$$

and for $-\lambda \pm \mu < 2$ and $a, b > 0$,

$$\begin{aligned}\int_0^\infty x^\lambda K_\mu(ax)\sin(bx)dx = {}& \frac{2^\lambda b\,\Gamma\big(\frac{2+\mu+\lambda}{2}\big)\Gamma\big(\frac{2+\lambda-\mu}{2}\big)}{a^{2+\lambda}}\\ &\times {}_2F_1\Big(\frac{2+\mu+\lambda}{2}, \frac{2+\lambda-\mu}{2}; \frac{3}{2}; -\frac{b^2}{a^2}\Big).\end{aligned} \tag{2.4}$$

Here, $\Gamma(\cdot)$ is the usual Gamma function, and ${}_2F_1$ is the hypergeometric function defined in (2.5) below.

2.2. Hypergeometric functions. For any real a, b, c with $c \neq 0, -1, -2, \ldots,$ the hypergeometric function is a power series defined by

$${}_2F_1(a, b; c; x) = \sum_{k=0}^\infty \frac{(a)_k (b)_k}{(c)_k}\frac{x^k}{k!} \quad \text{for } |x| < 1 \tag{2.5}$$

and by analytic continuation elsewhere (cf. [14, p. 1014] or [2, Chap. 2]). Here $(a)_k$ is the rising Pochhammer symbol, i.e.,

$$(a)_0 = 1, \quad (a)_k = a(a+1)\cdots(a+k-1) = \frac{\Gamma(a+k)}{\Gamma(a)}, \quad k \in \mathbb{N}.$$

It is known that the series ${}_2F_1(a, b; c; x)$ is absolutely convergent for all $|x| < 1$. Moreover, (i) if $c - a - b > 0$, the series ${}_2F_1(a, b; c; x)$ is absolutely convergent at $x = \pm 1$; (ii) if $-1 < c - a - b \le 0$, the series ${}_2F_1(a, b; c; x)$ is conditionally convergent at $x = -1$, but it is divergent at $x = 1$; (iii) if $c - a - b \le -1$, it diverges at $x = \pm 1$. Its divergent behavior at $x = 1$ can be characterized as follows (cf. [2, Chap. 2]):

- If $c = a + b$, then

$$\lim_{z\to 1^-} \frac{{}_2F_1(a, b; a+b; z)}{-\ln(1-z)} = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}. \tag{2.6}$$

- If $c < a + b$, then

$$\lim_{z\to 1^-} \frac{{}_2F_1(a, b; c; z)}{(1-z)^{c-a-b}} = \frac{\Gamma(c)\Gamma(a+b-c)}{\Gamma(a)\Gamma(b)}. \tag{2.7}$$

From the definition (2.5), we can easily obtain

$$\frac{d^k}{dx^k}{}_2F_1(a, b; c; x) = \frac{(a)_k(b)_k}{(c)_k}{}_2F_1(a+k, b+k; c+k; x).$$

According to [14, p. 1019], there holds

$$\begin{aligned}(2a-c-ax+bx)_2F_1(a,b;c;x)+(c-a)_2F_1(a-1,b;c;x)\\ +a(x-1)_2F_1(a+1,b;c;x)=0.\end{aligned} \tag{2.8}$$

We also recall the property of hypergeometric functions related to transformations of variable (cf. [29, p. 390]),

$$ {}_2F_1(a,b;c;x)=(1-x)^{-a}\,{}_2F_1\Big(a,c-b;c;\frac{x}{x-1}\Big), \tag{2.9}$$

and the Pfaff's formula on the linear transformation (cf. [2, (2.3.14)]): for integer $n\ge 0$,

$$ {}_2F_1(-n,b;c;x)=\frac{(c-b)_n}{(c)_n}{}_2F_1(-n,b;b-c-n+1;1-x). \tag{2.10}$$

Like (2.3)–(2.4), the following integral formulas (cf. [14, p. 825]) play a very important role in the algorithm development: for real $\mu>0$ and real $a,b,c>0$,

$$\int_0^\infty \cos(\mu x)_2F_1\Big(a,b;\frac{1}{2};-c^2x^2\Big)dx=2^{-a-b+1}\pi c^{-a-b}\mu^{a+b-1}\frac{K_{a-b}(\mu/c)}{\Gamma(a)\Gamma(b)}, \tag{2.11}$$

and for $a,b>1/2$,

$$\int_0^\infty x\sin(\mu x)_2F_1\Big(a,b;\frac{3}{2};-c^2x^2\Big)dx=2^{-a-b+1}\pi c^{-a-b}\mu^{a+b-2}\frac{K_{a-b}(\mu/c)}{\Gamma(a)\Gamma(b)}. \tag{2.12}$$

2.3. Gegenbauer polynomials. Gegenbauer polynomials, denoted by $C_n^\lambda(t)$, $t\in I:=(-1,1)$ and $\lambda>-1/2$, generalize Legendre and Chebyshev polynomials. They are defined by the three-term recurrence relation (cf. [14, p. 1000]):

$$\begin{aligned}&nC_n^\lambda(t)=2t(n+\lambda-1)C_{n-1}^\lambda(t)-(n+2\lambda-2)C_{n-2}^\lambda(t),\quad n\ge 2,\\ &C_0^\lambda(t)=1,\quad C_1^\lambda(t)=2\lambda t.\end{aligned} \tag{2.13}$$

They are orthogonal with respect to the weight function $\omega_\lambda(t)=(1-t^2)^{\lambda-1/2}$:

$$\int_{-1}^1 C_n^\lambda(t)C_m^\lambda(t)\omega_\lambda(t)\,dt=\gamma_n^\lambda\delta_{nm},\quad \gamma_n^\lambda=\frac{\pi 2^{1-2\lambda}\Gamma(n+2\lambda)}{n!\,(n+\lambda)\,\Gamma^2(\lambda)}. \tag{2.14}$$

The Gegenbauer polynomials can also be defined by the hypergeometric functions [14, p. 1000]:

$$\begin{aligned}C_{2n}^\lambda(t)&=\frac{(-1)^n}{(\lambda+n)B(\lambda,n+1)}\,{}_2F_1\Big(-n,n+\lambda;\frac{1}{2};t^2\Big),\\ C_{2n+1}^\lambda(t)&=\frac{(-1)^n2t}{B(\lambda,n+1)}\,{}_2F_1\Big(-n,n+\lambda+1;\frac{3}{2};t^2\Big),\end{aligned} \tag{2.15}$$

where $B(\cdot,\cdot)$ is the Beta function satisfying (cf. [14, p. 918]),

$$B(x,y)=\frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)}. \tag{2.16}$$

Using the linear transformation (2.10) and (2.15)–(2.16), we have

$$\begin{aligned} C_{2n}^{\lambda}(t) &= a_n^{\lambda}\, {}_2F_1\Big(-n, n+\lambda; \lambda+\frac{1}{2}; 1-t^2\Big), \\ C_{2n+1}^{\lambda}(t) &= b_n^{\lambda}\, t\, {}_2F_1\Big(-n, n+\lambda+1; \lambda+\frac{1}{2}; 1-t^2\Big), \end{aligned} \tag{2.17}$$

where

$$a_n^{\lambda} = \frac{(\lambda)_n}{(1)_n}\frac{\big(\lambda+\frac{1}{2}\big)_n}{\big(\frac{1}{2}\big)_n}, \quad b_n^{\lambda} = \frac{2\lambda\,(\lambda+1)_n}{(1)_n}\frac{\big(\lambda+\frac{1}{2}\big)_n}{\big(\frac{3}{2}\big)_n}. \tag{2.18}$$

Remark 2.1. Note that when $\lambda = 0$, we understand the classical Chebyshev polynomials in the sense of

$$T_n(t) = \frac{n}{2}\lim_{\lambda\to 0}\frac{C_n^{\lambda}(t)}{\lambda}, \quad n \geq 1.$$

Correspondingly, it follows from (2.17) that

$$T_{2n}(t) = {}_2F_1\Big(-n, n; \frac{1}{2}; 1-t^2\Big); \quad T_{2n+1}(t) = t\, {}_2F_1\Big(-n, n+1; \frac{1}{2}; 1-t^2\Big).$$

Here, we still denote $T_n(t) := C_n^0(t)$.

3. Fractional Laplacian of the modified mapped Gegenbauer functions.

In this section, we introduce the rational basis functions through the Gegenbauer polynomials with a singular mapping. For convenience, we call the resulting mapped basis, or modified mapped Gegenbauer functions, MMGFs, which differ from the usual mapped Gegenbauer functions by absorbing the weight function in the basis. We also present the explicit formulas for the evaluation of their fractional Laplacian, which plays an essential role in the spectral algorithms.

3.1. The mapping and MMGFs. Consider the one-to-one mapping between $t \in I = (-1,1)$ and $x \in \mathbb{R} = (-\infty, \infty)$ of the form

$$x = \frac{t}{\sqrt{1-t^2}} \quad \text{or} \quad t = \frac{x}{\sqrt{1+x^2}}, \quad t \in I, \ \ x \in \mathbb{R}. \tag{3.1}$$

It is clear that

$$1 - t^2 = \frac{1}{1+x^2}, \quad \frac{dx}{dt} = \frac{1}{(1-t^2)^{3/2}}. \tag{3.2}$$

DEFINITION 3.1. *For $\lambda > -1/2$, let $C_n^{\lambda}(t), t \in I = (-1,1)$, be the Gegenbauer polynomial of degree n as in* (2.13). *We define the MMGFs as*

$$R_n^{\lambda}(x) := \big(1+x^2\big)^{-\frac{\lambda+1}{2}} C_n^{\lambda}\Big(\frac{x}{\sqrt{1+x^2}}\Big), \quad x \in \mathbb{R}, \tag{3.3}$$

or equivalently,

$$R_n^{\lambda}(x) = S(t)C_n^{\lambda}(t), \quad S(t) := \sqrt{\omega_{\lambda}(t)\frac{dt}{dx}} = (1-t^2)^{\frac{\lambda+1}{2}}, \tag{3.4}$$

where x, t are associated with the mapping (3.1).

One verifies readily from (2.14) and (3.3)–(3.4) that

$$\int_{-\infty}^{\infty} R_n^\lambda(x) R_m^\lambda(x)\,dx = \gamma_n^\lambda \delta_{nm}, \tag{3.5}$$

where γ_n^λ is given in (2.14). Thanks to (2.13) and (3.3), the MMGFs satisfy the three-term recurrence relation:

$$\begin{aligned} &nR_n^\lambda(x) = \frac{2x}{\sqrt{1+x^2}}(n+\lambda-1)R_{n-1}^\lambda(x) - (n+2\lambda-2)R_{n-2}^\lambda(x), \quad n \ge 2;\\ &R_0^\lambda(x) = \frac{1}{(1+x^2)^{\frac{\lambda+1}{2}}}, \quad R_1^\lambda(x) = \frac{2\lambda x}{(1+x^2)^{1+\frac{\lambda}{2}}}. \end{aligned} \tag{3.6}$$

Moreover, we can show that

$$\lim_{x\to\infty} \left(1+x^2\right)^{\frac{\lambda+1}{2}} R_n^\lambda(x) = \frac{(2\lambda)_n}{n!}, \quad \lim_{x\to-\infty} \left(1+x^2\right)^{\frac{\lambda+1}{2}} R_n^\lambda(x) = (-1)^n \frac{(2\lambda)_n}{n!}.$$

It is clear that by (2.5), (2.17), and (3.2), we have

$$\begin{aligned} R_{2n}^\lambda(x) &= \frac{a_n^\lambda}{(1+x^2)^{\frac{\lambda+1}{2}}}\, {}_2F_1\Big(-n, n+\lambda; \lambda+\frac{1}{2}; \frac{1}{1+x^2}\Big)\\ &= a_n^\lambda \sum_{k=0}^{n} \frac{(-n)_k\,(n+\lambda)_k}{\big(\lambda+\frac12\big)_k\, k!} \frac{1}{(1+x^2)^{k+\frac{\lambda+1}{2}}}, \end{aligned} \tag{3.7}$$

and

$$\begin{aligned} R_{2n+1}^\lambda(x) &= \frac{b_n^\lambda}{(1+x^2)^{\frac{\lambda+1}{2}}} \frac{x}{\sqrt{1+x^2}}\, {}_2F_1\Big(-n, n+\lambda+1; \lambda+\frac{1}{2}; \frac{1}{1+x^2}\Big)\\ &= b_n^\lambda \sum_{k=0}^{n} \frac{(-n)_k\,(n+\lambda+1)_k}{\big(\lambda+\frac12\big)_k\, k!} \frac{x}{(1+x^2)^{k+\frac{\lambda}{2}+1}}. \end{aligned} \tag{3.8}$$

It is seen that the MMGFs are expressed in terms of

$$\frac{1}{(1+x^2)^\gamma} \ \text{ with } \ \gamma = k + \frac{\lambda+1}{2} \quad \text{or} \quad \frac{x}{(1+x^2)^\gamma} \ \text{ with } \ \gamma = k + \frac{\lambda}{2} + 1. \tag{3.9}$$

3.2. Formulas for computing fractional Laplacian of MMGFs. In view of (3.7)–(3.9), we first compute the fractional Laplacian of the simple functions in (3.9).

THEOREM 3.2. *For real $s > 0$, we have that for any $\gamma > 0$,*

$$(-\Delta)^s \Big\{ \frac{1}{(1+x^2)^\gamma} \Big\} = A_s^\gamma\, {}_2F_1\Big(s+\gamma, s+\frac12; \frac12; -x^2\Big), \tag{3.10}$$

and for any $\gamma > 1/2$,

$$(-\Delta)^s \Big\{ \frac{x}{(1+x^2)^\gamma} \Big\} = (2s+1) A_s^\gamma\; x\, {}_2F_1\Big(s+\gamma, s+\frac32; \frac32; -x^2\Big), \tag{3.11}$$

where the factor

$$A_s^\gamma := \frac{2^{2s}\Gamma(s+\gamma)\Gamma(s+\frac12)}{\sqrt{\pi}\,\Gamma(\gamma)}. \tag{3.12}$$

Proof. Recall the formula (cf. [29, 15.4.6])

$$ {}_2F_1(b,a;a;z) = (1-z)^{-b}. \tag{3.13} $$

Note that (3.13) also holds for $z<1$, with the analytic extension by the transformation formula (2.9) (see [14, 9.130]). Thus, we have

$$ v(x) := \frac{1}{(1+x^2)^\gamma} = {}_2F_1\Big(\gamma, \frac{1}{2}; \frac{1}{2}; -x^2\Big). \tag{3.14} $$

Then using (2.11) with $\mu=\xi, \alpha=\gamma$, and $\beta=1/2$, we obtain that for $\xi>0$,

$$ \begin{aligned} \hat{v}(\xi) := \mathscr{F}[v](\xi) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{e^{-\mathrm{i}x\xi}}{(1+x^2)^\gamma} dx = \frac{2}{\sqrt{2\pi}} \int_0^\infty \frac{\cos(x\xi)}{(1+x^2)^\gamma} dx \\ &= \sqrt{\frac{2}{\pi}} \int_0^\infty \cos(x\xi)\, {}_2F_1\Big(\gamma, \frac{1}{2}; \frac{1}{2}; -x^2\Big) dx \\ &= \sqrt{2\pi} 2^{-\gamma+\frac{1}{2}} \xi^{\gamma-\frac{1}{2}} \frac{K_{\gamma-\frac{1}{2}}(\xi)}{\Gamma(\gamma)\Gamma(\frac{1}{2})} = \frac{2^{1-\gamma}}{\Gamma(\gamma)} \xi^{\gamma-\frac{1}{2}} K_{\gamma-\frac{1}{2}}(\xi). \end{aligned} \tag{3.15} $$

Note that for $\xi<0$, we have $\hat{v}(\xi)=\hat{v}(-\xi)$. Consequently, from the definition (1.3) and (3.15), we obtain

$$ \begin{aligned} (-\Delta)^s v(x) &= \mathscr{F}^{-1}\big[|\xi|^{2s}\mathscr{F}[v](\xi)\big] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{\mathrm{i}x\xi} |\xi|^{2s} \hat{v}(\xi)\, d\xi \\ &= \frac{2^{1-\gamma}}{\sqrt{2\pi}\Gamma(\gamma)} \int_0^\infty \cos(x\xi)\, \xi^{2s+\gamma-\frac{1}{2}} K_{\gamma-\frac{1}{2}}(\xi)\, d\xi. \end{aligned} \tag{3.16} $$

Then using the formula (2.3) with $\lambda = 2s+\gamma-1/2, \mu=\gamma-1/2$, and $b=x$, we find

$$ (-\Delta)^s v(x) = \frac{2^{2s}\Gamma(s+\gamma)\Gamma(s+\frac{1}{2})}{\sqrt{\pi}\Gamma(\gamma)}\, {}_2F_1\Big(s+\gamma, s+\frac{1}{2}; \frac{1}{2}; -x^2\Big), \tag{3.17} $$

which yields (3.10).

The formula (3.11) can be derived in a similar fashion. Like (3.15), we obtain from (2.12) with $\mu=\xi, \alpha=\gamma$, and $\beta=3/2$ that for $\gamma>1/2$ and $\xi>0$,

$$ \begin{aligned} \mathscr{F}[xv](\xi) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{xe^{-\mathrm{i}x\xi}}{(1+x^2)^\gamma} dx = -\frac{2\mathrm{i}}{\sqrt{2\pi}} \int_0^\infty \frac{x\sin(x\xi)}{(1+x^2)^\gamma} dx \\ &= -\mathrm{i}\sqrt{\frac{2}{\pi}} \int_0^\infty x\sin(x\xi)\, {}_2F_1\Big(\gamma, \frac{3}{2}; \frac{3}{2}; -x^2\Big) dx \\ &= -\mathrm{i}\sqrt{2\pi} 2^{-\gamma-\frac{1}{2}} \xi^{\gamma-\frac{1}{2}} \frac{K_{\gamma-\frac{3}{2}}(\xi)}{\Gamma(\gamma)\Gamma(\frac{3}{2})} = -\mathrm{i}\frac{2^{1-\gamma}}{\Gamma(\gamma)} \xi^{\gamma-\frac{1}{2}} K_{\gamma-\frac{3}{2}}(\xi). \end{aligned} \tag{3.18} $$

Note that in this case, $\mathscr{F}[xv](-\xi) = -\mathscr{F}[xv](\xi)$. Similar to (3.16), we find

$$ \begin{aligned} (-\Delta)^s \big\{xv(x)\big\} &= \mathscr{F}^{-1}\big[|\xi|^{2s}\mathscr{F}[xv](\xi)\big] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{\mathrm{i}x\xi} |\xi|^{2s} \mathscr{F}[xv](\xi) d\xi \\ &= \frac{2^{2-\gamma}}{\sqrt{2\pi}\Gamma(\gamma)} \int_0^\infty \sin(x\xi) \xi^{2s+\gamma-\frac{1}{2}} K_{\gamma-\frac{3}{2}}(\xi)\, d\xi. \end{aligned} \tag{3.19} $$

Thus, we derive from (2.4) with $\lambda = 2s+\gamma-1/2, \mu = \gamma - 3/2$, and $b = x$ that

$$(3.20)\qquad (-\Delta)^s\big\{xv(x)\big\} = \frac{2^{2s+1}\Gamma(s+\gamma)\Gamma(s+3/2)}{\sqrt{\pi}\Gamma(\gamma)}\, x\, {}_2F_1\Big(s+\gamma, s+\frac{3}{2}; \frac{3}{2}; -x^2\Big).$$

Finally, the formula (3.11) follows from the property $\Gamma(z+1) = z\Gamma(z)$. ∎

Using the transformation formula (2.9), we can represent the formulas in Theorem 3.2 in terms of the hypergeometric function defined by the series in (2.5). Note that the former is more convenient for computation, while the latter is more suitable for analysis.

COROLLARY 3.3. *For real $s > 0$, we have that for any $\gamma > 0$,*

$$(3.21)\qquad (-\Delta)^s\Big\{\frac{1}{(1+x^2)^\gamma}\Big\} = \frac{A_s^\gamma}{(1+x^2)^{s+\gamma}}\, {}_2F_1\Big(-s, s+\gamma; \frac{1}{2}; \frac{x^2}{1+x^2}\Big),$$

and for any $\gamma > 1/2$,

$$(3.22)\qquad (-\Delta)^s\Big\{\frac{x}{(1+x^2)^\gamma}\Big\} = (2s+1)A_s^\gamma\, \frac{x}{(1+x^2)^{s+\gamma}}\, {}_2F_1\Big(-s, s+\gamma; \frac{3}{2}; \frac{x^2}{1+x^2}\Big),$$

where A_s^γ is defined as in (3.12).

Remark 3.1. It is seen that if s is a positive integer, then the hypergeometric functions in (3.21) and (3.22) become finite series. We can directly verify by using (2.5) that

$$(3.23)\qquad (-\Delta)^s\Big\{\frac{1}{(1+x^2)^\gamma}\Big\} \sim \frac{1}{(1+x^2)^{s+\gamma}},\quad (-\Delta)^s\Big\{\frac{x}{(1+x^2)^\gamma}\Big\} \sim \frac{x}{(1+x^2)^{s+\gamma}},$$

for $s = 1, 2, \dots,$ and $|x| \to \infty$. However, for noninteger $s > 0$, the hypergeometric functions may diverge as $|x| \to \infty$. Indeed, we find from (2.6) and (2.7) that

(i) if $\gamma = 1/2$, then

$$(3.24)\qquad (-\Delta)^s\Big\{\frac{1}{\sqrt{1+x^2}}\Big\} \sim \frac{\ln(1+x^2)}{(1+x^2)^{s+1/2}},$$

(ii) if $\gamma > 1/2$, then

$$(3.25)\qquad (-\Delta)^s\Big\{\frac{1}{(1+x^2)^\gamma}\Big\} \sim \frac{1}{(1+x^2)^{s+1/2}},$$

(iii) if $0 < \gamma < 1/2$, it has the same behavior as in (3.23).

Similarly, we can analyze the behavior at infinity for (3.22) for three cases: (i) $\gamma = 3/2$, (ii) $\gamma > 3/2$, and (iii) $1/2 < \gamma < 3/2$.

Remark 3.2. In a distinctive difference with the integer case, we see that the decay rate in the fractional case in (3.24) is independent of γ, if $\gamma > 1/2$.

With the above preparations, we are now ready to derive the explicit representation of the fractional Laplacian of $\{R_n^\lambda\}$.

THEOREM 3.4. *For real $s > 0$ and $\lambda > -1/2$, the fractional Laplacian of the MMGFs can be represented by*

$$(3.26)\qquad \begin{aligned}(-\Delta)^s R_{2n}^\lambda(x) &= a_n^\lambda \\ &\times \sum_{k=0}^{n} \frac{(-n)_k(n+\lambda)_k}{(\lambda+\frac{1}{2})_k\, k!} A_s^{k+\frac{\lambda+1}{2}}\, {}_2F_1\Big(s+k+\frac{\lambda+1}{2}, s+\frac{1}{2}; \frac{1}{2}; -x^2\Big)\end{aligned}$$

and

$$(-\Delta)^s R^\lambda_{2n+1}(x) = (2s+1)\, b^\lambda_n\, x \times \sum_{k=0}^{n} \frac{(-n)_k (n+\lambda+1)_k}{(\lambda+\frac12)_k k!}\, A_s^{k+\frac{\lambda}{2}+1}\, {}_2F_1\Big(s+k+\frac{\lambda}{2}+1, s+\frac32; \frac32; -x^2\Big), \tag{3.27}$$

where the constants a^λ_n, b^λ_n, *and* A^γ_s *are the same as in* (2.18) *and* (3.12).

Proof. By (3.7), we have

$$(-\Delta)^s R^\lambda_{2n}(x) = a^\lambda_n \sum_{k=0}^{n} \frac{(-n)_k (n+\lambda)_k}{(\lambda+\frac12)_k k!} (-\Delta)^s \Big\{ \frac{1}{(1+x^2)^{k+\frac{\lambda+1}{2}}} \Big\}, \tag{3.28}$$

so substituting (3.10) with $\gamma = k + \frac{\lambda+1}{2}$ into the above leads to (3.26).

Similarly, we derive from (3.8) that

$$(-\Delta)^s R^\lambda_{2n+1}(x) = b^\lambda_n \sum_{k=0}^{n} \frac{(-n)_k (n+\lambda+1)_k}{(\lambda+\frac12)_k k!} (-\Delta)^s \Big\{ \frac{x}{(1+x^2)^{k+\frac{\lambda}{2}+1}} \Big\}, \tag{3.29}$$

so substituting (3.11) with $\gamma = k + \frac{\lambda}{2} + 1$ into the above leads to (3.27). ∎

In view of the asymptotic results in Remark 3.1, we can analyze the decay rate of fractional Laplacian of the basis. Indeed, by virtue of (3.23)–(3.25), we obtain from (3.28)–(3.29) that (i) if $-1/2 < \lambda < 0$, then

$$(-\Delta)^s R^\lambda_{2n}(x) \sim \frac{1}{(1+x^2)^{s+\frac{\lambda+1}{2}}}; \tag{3.30}$$

(ii) if $\lambda = 0$, we have

$$(-\Delta)^s R^\lambda_{2n}(x) \sim \frac{\ln(1+x^2)}{(1+x^2)^{s+1/2}}; \tag{3.31}$$

(iii) if $\lambda > 0$, we have

$$(-\Delta)^s R^\lambda_{2n}(x) \sim \frac{1}{(1+x^2)^{s+1/2}}. \tag{3.32}$$

Similar results are also available for $(-\Delta)^s R^\lambda_{2n+1}(x)$. It is noteworthy from (3.3) and the above that the fractional Laplacian on the basis does not always lead to the gain in decay rate of $1/(1+x^2)^s$.

Remark 3.3. It is important to point out that the involved hypergeometric functions in (3.26) and (3.27) can be evaluated recursively by using (2.8). Denote

$$F_k(x) = {}_2F_1(a,b;c;-x^2), \quad a = s+k+\frac{\lambda+1}{2}, \;\; b = s+\frac12, \;\; c = \frac12.$$

Then by (2.8), we have

$$F_{k+1}(x) = \frac{c-a}{a(1+x^2)}\, F_{k-1}(x) + \frac{(2a-c)+(a-b)x^2}{a(1+x^2)} F_k(x) \tag{3.33}$$

for $k \ge 1$. Similarly, we can efficiently compute the hypergeometric functions in (3.27).

Remark 3.4. To enhance the resolution of the basis, one can also introduce a scaling parameter $\mu > 0$ (cf. [31]). More precisely, the algebraic mapping in (3.1) turns to

$$x = \frac{\mu\, t}{\sqrt{1-t^2}}, \quad t = \frac{x}{\sqrt{\mu^2+x^2}}.$$

The corresponding modified rational function can be defined as

$$R^{\lambda}_{n,\mu}(x) := \frac{\mu^{\lambda+\frac{1}{2}}}{(\mu^2+x^2)^{\frac{\lambda+1}{2}}} C^{\lambda}_n\Big(\frac{x}{\sqrt{\mu^2+x^2}}\Big) = \mu^{-\frac{1}{2}} R^{\lambda}_n\Big(\frac{x}{\mu}\Big).$$

In fact, it is straightforward to extend the previous properties and formulas to the scaled basis. For simplicity, we omit the details.

4. Estimates of MMGF approximation in fractional Sobolev spaces. In this section, we analyze the approximation property by the modified rational basis functions in fractional Sobolev spaces. We remark that there exist very limited results on the Legendre or Chebyshev rational approximations (see [16, 41, 33]). However, most of them are suboptimal. Here, we derive the optimal estimates in more general settings.

4.1. Fractional Sobolev spaces. For real $r \ge 0$, we define the fractional Sobolev space (as in [23, p. 30] and [1, Chap. 1])

$$H^r(\mathbb{R}) = \Big\{ u \in L^2(\mathbb{R}) : \int_{\mathbb{R}} (1+|\xi|^2)^r \big|\mathscr{F}[u](\xi)\big|^2 d\xi < +\infty \Big\}, \tag{4.1}$$

equipped with the norm

$$\|u\|_{H^r(\mathbb{R})} = \Big(\int_{\mathbb{R}} (1+|\xi|^2)^r \big|\mathscr{F}[u](\xi)\big|^2 d\xi \Big)^{1/2}. \tag{4.2}$$

We have the following space interpolation property (cf. [1, Chap. 1]).

LEMMA 4.1. *For real* $r_0, r_1 \ge 0$, *let* $r = (1-\theta)r_0 + \theta r_1$ *with* $\theta \in [0,1]$. *Then for any* $u \in H^{r_0}(\mathbb{R}) \cap H^{r_1}(\mathbb{R})$, *we have*

$$\|u\|_{H^r(\mathbb{R})} \le \|u\|^{1-\theta}_{H^{r_0}(\mathbb{R})} \|u\|^{\theta}_{H^{r_1}(\mathbb{R})}. \tag{4.3}$$

Proof. For the readers' reference, we sketch the derivation of this interpolation property. It is clear that by (4.2),

$$\begin{aligned}\|u\|^2_{H^r(\mathbb{R})} &= \int_{\mathbb{R}} (1+|\xi|^2)^{(1-\theta)r_0+\theta r_1} |\mathscr{F}[u](\xi)|^2 d\xi \\ &= \int_{\mathbb{R}} \Big\{ (1+|\xi|^2)^{(1-\theta)r_0} |\mathscr{F}[u](\xi)|^{2(1-\theta)} \Big\} \Big\{ (1+|\xi|^2)^{\theta r_1} |\mathscr{F}[u](\xi)|^{2\theta} \Big\} d\xi.\end{aligned}$$

Using the Hölder's inequality with $p = 1/(1-\theta)$ and $q = 1/\theta$, we obtain

$$\begin{aligned}\|u\|^2_{H^r(\mathbb{R})} &\le \Big\{ \int_{\mathbb{R}} (1+|\xi|^2)^{r_0} |\mathscr{F}[u](\xi)|^2 d\xi \Big\}^{1-\theta} \Big\{ \int_{\mathbb{R}} (1+|\xi|^2)^{r_1} |\mathscr{F}[u](\xi)|^2 d\xi \Big\}^{\theta} \\ &= \|u\|^{2(1-\theta)}_{H^{r_0}(\mathbb{R})} \|u\|^{2\theta}_{H^{r_1}(\mathbb{R})}.\end{aligned}$$

This completes the proof. ∎

4.2. Error estimate of orthogonal projections. Define the approximation space

$$V_N^\lambda = \{\phi(x) : \phi(x) = S(t)P(t) \ \ \forall P \in \mathcal{P}_N\} = \mathrm{span}\{R_n^\lambda(x) : n = 0, 1, \ldots, N\}. \tag{4.4}$$

Consider the L^2-orthogonal projection $\pi_N^\lambda : L^2(\mathbb{R}) \to V_N^\lambda$, i.e.,

$$\pi_N^\lambda u(x) = \sum_{n=0}^{N} \hat{u}_n^\lambda R_n^\lambda(x), \qquad \hat{u}_n^\lambda = \frac{1}{\gamma_n^\lambda} \int_{\mathbb{R}} u(x) R_n^\lambda(x) dx. \tag{4.5}$$

For notational convenience, we introduce the pairs of functions associated with the mapping (3.1):

$$\begin{aligned} &u(x) = U(t(x)), \quad \breve{u}(x) = \frac{u(x)}{s(x)} = \frac{U(t)}{S(t)} = \breve{U}(t), \quad \text{where} \\ &s(x) := \frac{1}{(1+x^2)^{(\lambda+1)/2}} = (1-t^2)^{(\lambda+1)/2} := S(t). \end{aligned} \tag{4.6}$$

In what follows, the notation with or without " $\breve{}$ " has the same meaning.

In order to describe the approximation errors, we introduce new differential operators as follows:

$$\begin{aligned} &\mathscr{D}_x u := a(x)\frac{d\breve{u}}{dx} = \frac{d\breve{U}}{dt}, \quad \mathscr{D}_x^2 u := a(x)\frac{d}{dx}\Big\{a(x)\frac{d\breve{u}}{dx}\Big\} = \frac{d^2\breve{U}}{dt^2}, \ldots, \\ &\mathscr{D}_x^k u = a(x)\frac{d}{dx}\Big\{a(x)\frac{d}{dx}\Big\{\cdots\Big\{a(x)\frac{d\breve{u}}{dx}\Big\}\cdots\Big\}\Big\} = \frac{d^k\breve{U}}{dt^k}, \end{aligned} \tag{4.7}$$

where $a(x) = dx/dt = (1+x^2)^{\frac{3}{2}}$. Correspondingly, we define the Sobolev space

$$\mathbb{B}_\lambda^m(\mathbb{R}) = \big\{u : u \text{ is measurable in } \mathbb{R} \text{ and } \|u\|_{\mathbb{B}_\lambda^m(\mathbb{R})} < \infty\big\}, \tag{4.8}$$

equipped with the norm and seminorm

$$\begin{aligned} &\|u\|_{\mathbb{B}_\lambda^m(\mathbb{R})} = \Big(\sum_{k=0}^{m} \big\|(1+x^2)^{-\frac{\lambda+m+1}{2}} \mathscr{D}_x^k u\big\|_{L^2(\mathbb{R})}^2\Big)^{\frac{1}{2}}, \\ &|u|_{\mathbb{B}_\lambda^m(\mathbb{R})} = \big\|(1+x^2)^{-\frac{\lambda+m+1}{2}} \mathscr{D}_x^m u\big\|_{L^2(\mathbb{R})}. \end{aligned} \tag{4.9}$$

THEOREM 4.2. *For any* $u \in H^s(\mathbb{R}) \cap \mathbb{B}_\lambda^m(\mathbb{R})$ *with integer* $1 \le m \le N+1$, $s \in (0,1)$, *and* $\lambda > -1/2$, *we have*

$$\|\pi_N^\lambda u - u\|_{H^s(\mathbb{R})} \le cN^{s-m} |u|_{\mathbb{B}_\lambda^m(\mathbb{R})}, \tag{4.10}$$

where c *is a positive constant independent of* N *and* u.

Proof. We take two steps to carry out the proof.

Step 1. We first prove that

$$\big\|\sqrt{1+x^2}\,(\pi_N^\lambda u - u)'\big\|_{L^2(\mathbb{R})} + N\|\pi_N^\lambda u - u\|_{L^2(\mathbb{R})} \le cN^{1-m} |u|_{\mathbb{B}_\lambda^m(\mathbb{R})}. \tag{4.11}$$

For this purpose, we study the close relation between π_N^λ and the orthogonal projection $\varPi_N^\lambda : L^2_{\omega_\lambda}(I) \to \mathcal{P}_N$, such that for any $\varPhi \in L^2_{\omega_\lambda}(I)$,

$$\int_{-1}^{1} (\varPi_N^\lambda \varPhi(t) - \varPhi(t))\varPsi(t)\omega_\lambda(t)\,dt = 0 \quad \forall \varPsi \in \mathcal{P}_N. \tag{4.12}$$

Recall the Gegenbauer polynomial approximation result (cf. [31, Thm. 3.35]): *if* $\varPhi^{(l)}(t) \in L^2_{\omega_{\lambda+l}}(I)$ *for* $0 \le l \le m$, *we have*

$$\|(\varPi_N^\lambda \varPhi - \varPhi)^{(l)}\|_{L^2_{\omega_{\lambda+l}}(I)} \le cN^{l-m}\|\varPhi^{(m)}\|_{L^2_{\omega_{\lambda+m}}(I)}, \tag{4.13}$$

where the weight function $\omega_a(t) = (1-t^2)^{(a+1)/2}$.

From (4.5) and (4.6), we find

$$\begin{aligned} \hat{u}_n &= \frac{1}{\gamma_n^\lambda}\int_{\mathbb{R}} u(x)R_n^\lambda(x)dx = \frac{1}{\gamma_n^\lambda}\int_{-1}^{1} U(t)S(t)C_n^\lambda(t)\frac{dx}{dt}dt \\ &= \frac{1}{\gamma_n^\lambda}\int_{-1}^{1}\frac{U(t)}{S(t)}C_n^\lambda(t)(1-t^2)^{\lambda-1/2}dt = \frac{1}{\gamma_n^\lambda}\int_{-1}^{1}\breve{U}(t)C_n^\lambda(t)\omega_\lambda(t)dt = \widehat{\breve{U}}_n. \end{aligned} \tag{4.14}$$

Therefore, we have

$$\begin{aligned} e_N(x) := u(x) - \pi_N^\lambda u(x) &= \sum_{n=N+1}^{\infty}\hat{u}_n R_n^\lambda(x) = S(t)\sum_{n=N+1}^{\infty}\widehat{\breve{U}}_n C_n^\lambda(t) \\ &= S(t)\big(\breve{U}(t) - \varPi_N^\lambda\breve{U}(t)\big) := S(t)\breve{e}_N(t). \end{aligned} \tag{4.15}$$

As a result, there holds

$$\int_{\mathbb{R}} |e_N(x)|^2 dx = \int_{-1}^{1}|S(t)\breve{e}_N(t)|^2\frac{dx}{dt}dt = \int_{-1}^{1}|\breve{e}_N(t)|^2\omega_\lambda(t)dt. \tag{4.16}$$

Thus, using (4.13) with $l = 0$, we derive from (4.7)–(4.9) that

$$\|e_N\|_{L^2(\mathbb{R})} = \|\breve{e}_N\|_{L^2_{\omega_\lambda}(I)} \le cN^{-m}\|\partial_t^m\breve{U}\|_{L^2_{\omega_{\lambda+m}}(I)} = cN^{-m}|u|_{\mathbb{B}_\lambda^m(\mathbb{R})}. \tag{4.17}$$

Like (4.15), we can show

$$\begin{aligned} e_N'(x) &= \sum_{n=N+1}^{\infty}\hat{u}_n\frac{dR_n^\lambda}{dx}(x) = \sum_{n=N+1}^{\infty}\widehat{\breve{U}}_n\frac{d}{dt}\big(S(t)C_n^\lambda(t)\big)\frac{dt}{dx} \\ &= \big(S(t)\breve{e}_N'(t) + S'(t)\breve{e}_N(t)\big)\frac{dt}{dx} \\ &= (1-t^2)^{\frac{\lambda}{2}+2}\breve{e}_N'(t) - (\lambda+1)t(1-t^2)^{\frac{\lambda}{2}+1}\breve{e}_N(t). \end{aligned} \tag{4.18}$$

Similar to (4.16), we derive from (4.13) with $l = 0, 1$ that

$$\begin{aligned} \int_{\mathbb{R}}|e_N'(x)|^2(1+x^2)dx &\le 2\int_{-1}^{1}|\breve{e}_N'(t)|^2\omega_{\lambda+2}(t)dt + 2(1+\lambda)^2\int_{-1}^{1}|\breve{e}_N(t)|^2\omega_\lambda(t)dt \\ &\le cN^{2-2m}\|\partial_t^m\breve{U}\|^2_{L^2_{\omega_{\lambda+m}}(I)} = cN^{2-2m}|u|^2_{\mathbb{B}_\lambda^m(\mathbb{R})}. \end{aligned}$$

Then the estimate (4.11) is a direct consequence of (4.17) and the above.

Step 2. It is evident that the result (4.11) implies

$$\begin{aligned}\|\pi_N^\lambda u-u\|_{H^1(\mathbb{R})} &\le \big\|\sqrt{1+x^2}\,(\pi_N^\lambda u-u)'\big\|_{L^2(\mathbb{R})}+\|\pi_N^\lambda u-u\|_{L^2(\mathbb{R})}\\ &\le cN^{1-m}|u|_{\mathbb{B}_\lambda^m(\mathbb{R})},\end{aligned} \tag{4.19}$$

and

$$\|\pi_N^\lambda u-u\|_{L^2(\mathbb{R})}\le cN^{-m}|u|_{\mathbb{B}_\lambda^m(\mathbb{R})}. \tag{4.20}$$

Then using the interpolation inequality in Lemma 4.1 with $r_0=0, r_1=1$, and $\theta=s$, we obtain from (4.19)–(4.20) that

$$\|\pi_N^\lambda u-u\|_{H^s(\mathbb{R})}\le \|\pi_N^\lambda u-u\|_{L^2(\mathbb{R})}^{1-s}\,\|\pi_N^\lambda u-u\|_{H^1(\mathbb{R})}^{s}\le cN^{s-m}|u|_{\mathbb{B}_\lambda^m(\mathbb{R})}. \tag{4.21}$$

This completes the proof. ∎

In the error analysis, it is necessary to consider the H^s-orthogonal projection. Define the bilinear form on $H^s(\mathbb{R})$:

$$a_s(u,v)=\big((-\Delta)^{s/2}u,(-\Delta)^{s/2}v\big)+(u,v). \tag{4.22}$$

Consider the orthogonal projection $\pi_{N,\lambda}^s: H^s(\mathbb{R})\to V_N^\lambda$ such that

$$a_s(\pi_{N,\lambda}^s u-u,v)=0\quad \forall\, v\in V_N^\lambda. \tag{4.23}$$

Then by the property of the orthogonal projection operator, we have

$$\|\pi_{N,\lambda}^s u-u\|_{H^s(\mathbb{R})}=\inf_{\phi\in V_N^\lambda}\|\phi-u\|_{H^s(\mathbb{R})}. \tag{4.24}$$

Taking $\phi=\pi_N^\lambda u$, we immediately derive the following estimate.

THEOREM 4.3. *For any $u\in H^s(\mathbb{R})\cap\mathbb{B}_\lambda^m(\mathbb{R})$ with integer $1\le m\le N+1$, $s\in(0,1)$, and $\lambda>-1/2$, we have*

$$\|\pi_{N,\lambda}^s u-u\|_{H^s(\mathbb{R})}\le cN^{s-m}|u|_{\mathbb{B}_\lambda^m(\mathbb{R})}, \tag{4.25}$$

where c is a positive constant independent of N and u.

4.3. Error estimate of interpolation. Let $\{t_j^\lambda,\rho_j^\lambda\}_{j=0}^N$ be the Gegenbauer–Gauss quadrature nodes and weights, where $\{t_j^\lambda\}$ are zeros of the Gegenbauer polynomial $C_{N+1}^\lambda(t)$. Define the mapped nodes and weights:

$$x_j^\lambda=\frac{t_j^\lambda}{\sqrt{1-(t_j^\lambda)^2}},\quad \omega_j^\lambda=(1+(t_j^\lambda)^2)^{-\lambda}\rho_j^\lambda,\quad 0\le j\le N. \tag{4.26}$$

Then by the exactness of the Gagenbauer–Gauss quadrature (cf. [31, Chap. 3]), we have

$$\begin{aligned}\int_{\mathbb{R}}u(x)v(x)\,dx &=\int_{-1}^1\frac{U(t)V(t)}{(1-t^2)^{3/2}}dt=\int_{-1}^1\frac{U(t)}{S(t)}\frac{U(t)}{S(t)}(1-t^2)^{\lambda-1/2}dt\\ &=\sum_{j=0}^N\frac{U(t_j^\lambda)}{S(t_j^\lambda)}\frac{V(t_j^\lambda)}{S(t_j^\lambda)}\rho_j^\lambda,\qquad \text{if}\quad \frac{U(t)}{S(t)}\cdot\frac{V(t)}{S(t)}\in\mathcal{P}_{2N+1},\end{aligned}$$

which, together with (4.4), implies the exactness of quadrature

$$\int_{\mathbb{R}} u(x)v(x)\,dx = \sum_{j=0}^{N} u(x_j^\lambda)v(x_j^\lambda)\omega_j^\lambda \quad \forall\, u\cdot v \in V_{2N+1}^\lambda. \tag{4.27}$$

We now introduce the interpolation operator $I_N^\lambda u : C(\mathbb{R}) \to V_N^\lambda$ such that

$$I_N^\lambda u(x_j^\lambda) = u(x_j^\lambda), \quad 0 \le j \le N.$$

As a consequence of (3.5) and (4.27), we have

$$I_N^\lambda u(x) = \sum_{n=0}^{N} \tilde{u}_n^\lambda R_n^\lambda(x), \quad \text{where} \quad \tilde{u}_n^\lambda = \frac{1}{\gamma_n^\lambda}\sum_{j=0}^{N} u(x_j^\lambda)R_n^\lambda(x_j^\lambda)\omega_j^\lambda. \tag{4.28}$$

We have the following interpolation approximation result.

THEOREM 4.4. *For any $u \in H^s(\mathbb{R})\cap\mathbb{B}_\lambda^m(\mathbb{R})$ with integer $1 \le m \le N+1$, $s \in (0,1)$, and $\lambda > -1/2$, we have*

$$\|I_N^\lambda u - u\|_{H^s(\mathbb{R})} \le cN^{s-m}|u|_{\mathbb{B}_\lambda^m(\mathbb{R})}, \tag{4.29}$$

where c is a positive constant independent of N and u.

Proof. Recall the Gegenbauer–Gauss interpolation $I_N^G : C(-1,1) \to \mathcal{P}_N$, such that

$$I_N^G U(t_j^\lambda) = U(t_j^\lambda), \quad 0 \le j \le N.$$

Then we have the expansion

$$I_N^G U(t) = \sum_{n=0}^{N} \tilde{U}_n^\lambda C_n^\lambda(t), \quad \text{where} \quad \tilde{U}_n^\lambda = \frac{1}{\gamma_n^\lambda}\sum_{j=0}^{N} U(t_j^\lambda)C_n^\lambda(t_j^\lambda)\rho_j^\lambda. \tag{4.30}$$

One verifies from (3.3), (4.6), (4.26), and (4.28)–(4.30) that

$$I_N^\lambda u(x) = S(t)\, I_N^G\Big\{\frac{U(t)}{S(t)}\Big\} = S(t)\, I_N^G \breve{U}(t). \tag{4.31}$$

Thus,

$$e_N(x) := u(x) - I_N^\lambda u(x) = S(t)\big(\breve{U}(t) - I_N^G\breve{U}(t)\big) := S(t)\breve{e}_N(t), \tag{4.32}$$

where with a little abuse of notation, we still use the same notation as in (4.15). Following the lines as in (4.16)–(4.2), we can show that

$$\|I_N^\lambda u - u\|_{L^2(\mathbb{R})} = \|I_N^G\breve{U} - \breve{U}\|_{L^2_{\omega_\lambda}(I)} \tag{4.33}$$

and

$$\|(I_N^\lambda u - u)'\|_{L^2(\mathbb{R})} \le c\big(\|I_N^G\breve{U} - \breve{U}\|_{L^2_{\omega_\lambda}(I)} + \|\sqrt{1-t^2}(I_N^G\breve{U} - \breve{U})'\|_{L^2_{\omega_\lambda}(I)}\big). \tag{4.34}$$

According to [31, Thm. 3.41] on the Gegenbauer–Gauss interpolation error estimate, we have

$$N\|I_N^G\breve{U}-\breve{U}\|_{L^2_{\omega_\lambda}(I)}+\|\sqrt{1-t^2}(I_N^G\breve{U}-\breve{U})'\|_{L^2_{\omega_\lambda}(I)} \\ \le cN^{1-m}\|\partial_t^m\breve{U}\|_{L^2_{\omega_{\lambda+m}}(I)}.$$

Then by the interpolation inequality in Lemma 4.1, we obtain from the above that

$$\|I_N^\lambda u-u\|_{H^s(\mathbb{R})}\le\|I_N^\lambda u-u\|^{1-s}_{L^2(\mathbb{R})}\,\|I_N^\lambda u-u\|^s_{H^1(\mathbb{R})}\le cN^{s-m}|u|_{\mathbb{B}^m_\lambda(\mathbb{R})}.$$

This completes the proof. ∎

5. Modified rational spectral-Galerkin methods.

In this section, we consider the spectral-Galerkin approximation to a model equation and conduct the error analysis. We also present some numerical results to show our proposed method outperforms the Hermite approximations in [28, 39].

5.1. The scheme and its convergence.

Consider the model equation

$$\begin{cases}(-\Delta)^{\alpha/2}u(x)+\rho u(x)=f(x), & x\in\mathbb{R},\\ u(x)\to 0, & |x|\to\infty,\end{cases} \tag{5.1}$$

for $\alpha\in(0,2)$, where $f\in L^2(\mathbb{R})$ and the constant $\rho>0$.

For notational convenience, let $s=\alpha/2$. A weak form of (5.1) is to find $u\in H^s(\mathbb{R})$ such that

$$\tilde{a}_s(u,v):=\big((-\Delta)^{s/2}u,(-\Delta)^{s/2}v\big)+\rho(u,v)=(f,v)\quad\forall v\in H^s(\mathbb{R}). \tag{5.2}$$

The spectral-Galerkin scheme is to find $u_N\in V_N^\lambda$ (defined in (4.4)) such that

$$\tilde{a}_s(u_N,v_N)=(I_N^\lambda f,v_N)\quad\forall v_N\in V_N^\lambda. \tag{5.3}$$

Denote $e_N=u_N-\pi^s_{N,\lambda}u$ and $\tilde{e}_N=u-\pi^s_{N,\lambda}u$. By a standard analysis, we find that for any $v_N\in V_N^\lambda$,

$$\begin{aligned}\tilde{a}_s(e_N,v_N)&=\tilde{a}_s(\tilde{e}_N,v_N)+(I_N^\lambda f-f,v_N)\\&=a_s(\tilde{e}_N,v_N)+(\rho-1)(\tilde{e}_N,v_N)+(I_N^\lambda f-f,v_N)\\&=(\rho-1)(\tilde{e}_N,v_N)+(I_N^\lambda f-f,v_N).\end{aligned}$$

Taking $v_N=e_N$ and using the Cauchy–Schwarz inequality, we obtain

$$\|e_N\|^2_{H^s(\mathbb{R})}\le c\big(\|\tilde{e}_N\|^2_{L^2(\mathbb{R})}+\|I_N^\lambda f-f\|^2_{L^2(\mathbb{R})}\big).$$

Thus, by the triangle inequality, we derive

$$\begin{aligned}\|u-u_N\|_{H^s(\mathbb{R})}&\le c\big(\|\tilde{e}_N\|_{H^s(\mathbb{R})}+\|I_N^\lambda f-f\|_{L^2(\mathbb{R})}\big)\\&\le cN^{s-m}|u|_{\mathbb{B}^m_\lambda(\mathbb{R})}+cN^{-k}|f|_{\mathbb{B}^k_\lambda(\mathbb{R})}.\end{aligned} \tag{5.4}$$

In summary, we have the following convergence result.

THEOREM 5.1. *For any $u\in H^s(\mathbb{R})\cap\mathbb{B}^m_\lambda(\mathbb{R})$ and $f\in\mathbb{B}^k_\lambda(\mathbb{R})$ with integer $1\le m,k\le N+1$, $s=\alpha/2\in(0,1)$, and $\lambda>-1/2$, we have*

$$\|u-u_N\|_{H^s(\mathbb{R})}\le cN^{s-m}|u|_{\mathbb{B}^m_\lambda(\mathbb{R})}+cN^{-k}|f|_{\mathbb{B}^k_\lambda(\mathbb{R})}, \tag{5.5}$$

where c is a positive constant independent of N and u,f.

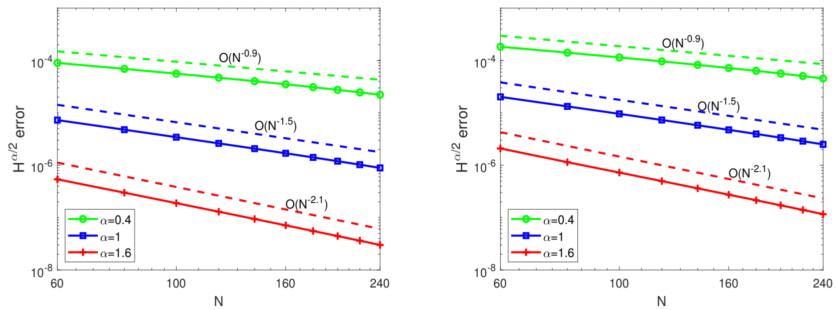

FIG. 1. *$H^{\alpha/2}$-error with MMGFs with $\lambda = 0$. Left: $u_e(x) = \exp(-x^2)$ with scaling factor $\mu = 5$. Right: $u_a(x) = (1 + x^2)^{-2.3}$ with scaling factor $\mu = 3$.*

5.2. Numerical examples. We now present several examples to show the convergence behavior of the above spectral Galerkin method. In all tests, we report the numerical errors in the discrete $H^{\alpha/2}$-norm and set $\rho = 1$. Here, we only consider the cases with $\lambda = 0$ and $\lambda = 0.5$, which correspond to the modified mapped Chebyshev rational functions and modified mapped Legendre functions, respectively.

Example 1: *Accuracy test for given exact solutions.* Consider (5.1) with the following exact solutions:

$$u_e(x) = \exp(-x^2), \quad u_a(x) = (1 + x^2)^{-r}, \quad r > 0.$$

It is known from [39] and (3.10) that source terms are respectively

$$f_e(x) = \rho \exp(-x^2) + \frac{2^\alpha \Gamma(\frac{\alpha+1}{2})}{\Gamma(\frac{1}{2})}\, {}_1F_1\Big(\frac{\alpha+1}{2}; \frac{1}{2}; -x^2\Big),$$
$$f_a(x) = \rho(1 + x^2)^{-r} + \frac{2^\alpha \Gamma(\frac{\alpha}{2} + r)\Gamma(\frac{\alpha+1}{2})}{\Gamma(r)\Gamma(\frac{1}{2})}\, {}_2F_1\Big(\frac{\alpha}{2} + r, \frac{\alpha+1}{2}; \frac{1}{2}; -x^2\Big).$$

In Figure 1, we plot the errors measured by the discrete $H^{\alpha/2}$-norm the above exact solutions. Using the property of confluent hypergeometric function, we find $f_e(x) \sim (1 + x^2)^{\frac{\alpha+1}{2}}$. Thus, the error is dominated by the interpolation error of the source term. In fact, from Theorem 5.1 and with direct calculation, we can find the convergence rate is of order $O(N^{-(\alpha+\frac{1}{2})})$, so an algebraic decay of the error is expected, which agrees well with the numerical results. Similarly, for the exact solution u_a, we find $f_e(x) \sim (1 + x^2)^{\min(r, \frac{\alpha+1}{2})}$. When $r = 2.3$, the error is also dominated by the interpolation error of the right-hand side. Thus, the same convergence rate is obtained as with the former case.

Example 2: *Exponential decaying* $f(x)$. We first consider (5.1) with $f(x) = \exp(-x^2/2)(1 + x)$. Since the closed-form exact solution is not available, we take the numerical solution with $N = 600$ as the reference solution. The convergence results with MMGFs for $\alpha = 0.4, 1, 1.6$ are presented in Figure 2 (middle and right). In the left plot, we have also presented the convergence results for the Hermite function approach in [28]. It is clearly seen that the MMGF approach outperforms the Hermite approximations for all cases, namely, the MMGF approach admits much higher convergence rates. This can also be seen from Table 1, where we have presented the order of convergence for both approaches.

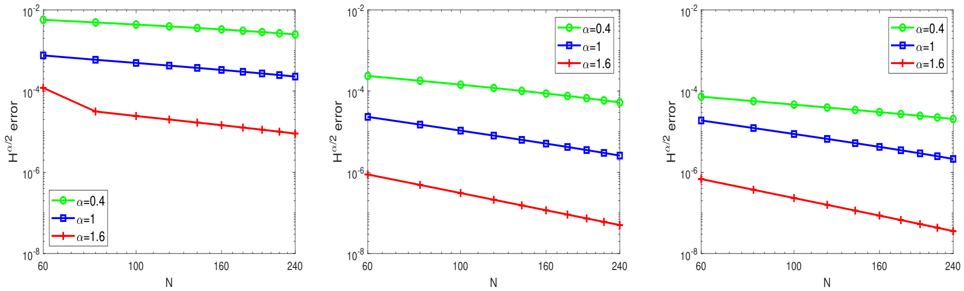

Fig. 2. *$H^{\alpha/2}$-error with $f(x) = \exp(-x^2/2)(1+x)$. Left: Hermite function approach in* [28] *with scaling factor* $1/0.4$. *Middle: MMGF approach with $\lambda = 0$ and scaling factor $\mu = 5$. Right: MMGF approach with $\lambda = 0.5$ and scaling factor $\mu = 5$.*

Table 1

Rate of convergence using the generalized Hermite function, MMGFs with $\lambda = 0$, and MMGFs with $\lambda = 0.5$, $\alpha = 1$, and $f(x) = \exp(-x^2/2)(1+x)$.

	Hermite		MMGF $\lambda = 0$		MMGF $\lambda = 0.5$	
N	$H^{\alpha/2}$-error	Order	$H^{\alpha/2}$-error	Order	$H^{\alpha/2}$-error	Order
60	7.58e-4	–	2.32e-5	–	1.90e-5	–
80	5.93e-4	0.86	1.50e-5	1.52	1.23e-5	1.50
100	4.95e-4	0.81	1.06e-5	1.53	8.80e-6	1.51
120	4.26e-4	0.82	8.03e-6	1.55	6.66e-6	1.53
140	3.74e-4	0.84	6.31e-6	1.57	5.24e-6	1.56
160	3.33e-4	0.86	5.10e-6	1.59	4.24e-6	1.59
180	3.00e-4	0.89	4.21e-6	1.62	3.50e-6	1.62
200	2.72e-4	0.92	3.54e-6	1.66	2.94e-6	1.66
220	2.49e-4	0.95	3.01e-6	1.70	2.50e-6	1.71
240	2.28e-4	0.98	2.58e-6	1.75	2.14e-6	1.77

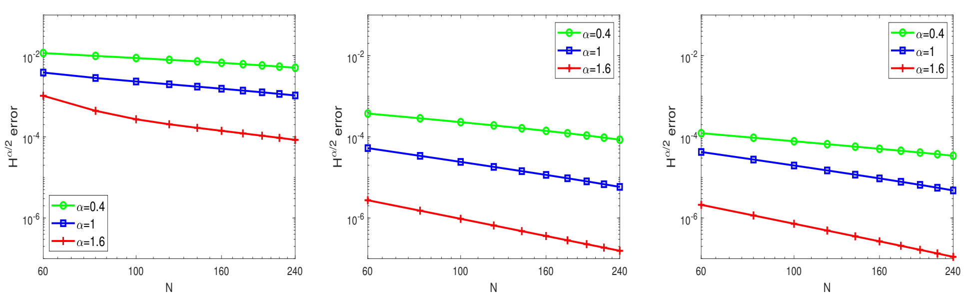

Fig. 3. *$H^{\alpha/2}$-error with $f(x) = \frac{1}{(1+x^2)^2}$. Left: Hermite function approach in* [28] *with scaling factor* $1/0.7$. *Middle: The MMGF approach with $\lambda = 0$ and scaling factor $\mu = 3$. Right: The MMGF approach with $\lambda = 0.5$ and scaling factor $\mu = 3$.*

Example 3: *Algebraic decaying $f(x)$.* We next consider (5.1) with an algebraic decay source term: $f(x) = \frac{1}{(1+x^2)^2}$. The plots of the error decay for both Hermite functions and MMGFs are in Figure 3. Indeed, we observe the convergence behavior similar to the previous example—the MMGF approach has a much better performance. The comparison in Table 2 also shows that the proposed approach converges much faster than the Hermite method.

Table 2

Rate of convergence using the generalized Hermite function, MMGF with $\lambda = 0$, and MMGF with $\lambda = 0.5$. $\alpha = 1$, and $f(x) = \frac{1}{(1+x^2)^2}$.

	Hermite		MMGF $\lambda = 0$		MMGF $\lambda = 0.5$	
N	$H^{\alpha/2}$-error	Order	$H^{\alpha/2}$-error	Order	$H^{\alpha/2}$-error	Order
60	3.83e-3	–	5.28e-5	–	4.24e-5	–
80	2.82e-3	1.07	3.40e-5	1.53	2.76e-5	1.49
100	2.31e-3	0.90	2.41e-5	1.54	1.97e-5	1.51
120	1.97e-3	0.86	1.82e-5	1.55	1.49e-5	1.53
140	1.72e-3	0.87	1.43e-5	1.57	1.17e-5	1.56
160	1.53e-3	0.88	1.15e-5	1.59	9.47e-6	1.59
180	1.38e-3	0.90	9.54e-6	1.62	7.83e-6	1.62
200	1.25e-3	0.93	8.01e-6	1.66	6.57e-6	1.66
220	1.14e-3	0.96	6.81e-6	1.70	5.58e-6	1.71
240	1.05e-3	1.00	5.85e-6	1.75	4.78e-6	1.77

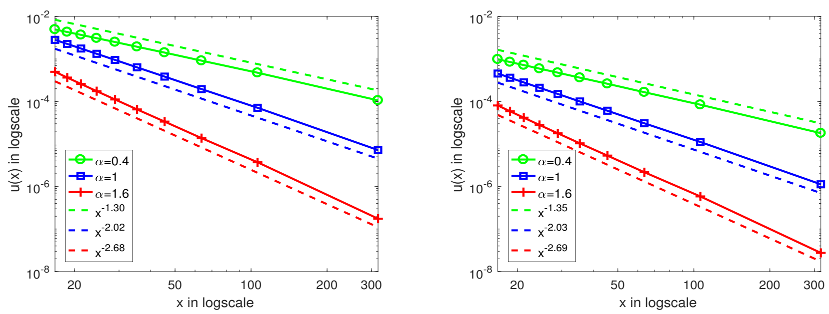

Fig. 4. *Asymptotic behavior of $u(x)$ with different α. Left: $f(x) = \exp(-x^2/2)(1 + x)$. Right: $f(x) = \frac{1}{(1+x^2)^2}$.*

To better understand the solution behaviors, we present in Figure 4 the asymptotic behavior of the "exact" solutions as $|x| \gg 1$ for the above two examples. We see that, for both examples with very different decay of $f(x)$, the solution $u(x)$ decays at the same rate: $|x|^{-\alpha-1}$. This shows that the solution decays at the rate of a power law, as opposite to the usual Laplacian. This also explains the reason why MMGFs have a better performance than the Hermite functions.

6. Modified rational spectral collocation methods. With the formulas in Theorem 3.4 at our disposal, we can directly generate the spectral fractional differentiation matrices and develop direct collocation methods as with the Hermite collocation methods in [39] for one-dimensional fractional equations. However, it seems nontrivial and largely open to analyze its convergence. In fact, we can also implement the collocation method in the Fourier transformed domain (cf. [28]), which turns out more natural for extending the method to multiple dimensions (see subsection 7 below).

6.1. Fractional differentiation matrices. Let $\{x_j^\lambda, \omega_j^\lambda\}_{j=0}^N$ be the mapped Gegenbauer–Gauss collocation points and weights as given in (4.26). For any $u_N \in V_N^\lambda$, we write

$$u_N(x) = \sum_{j=0}^{N-1} u_j l_j(x), \quad \text{with} \quad l_j(x_k^\lambda) = \delta_{jk}, \quad 0 \le j, k \le N-1,$$

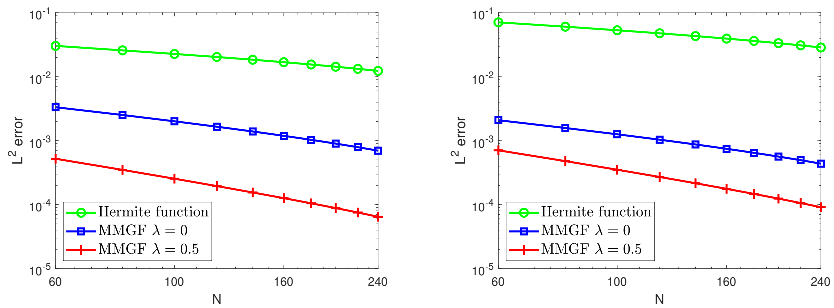

FIG. 5. *Numerical results for the multiterm fractional model. Left:* $f(x) = \exp(-\frac{x^2}{2})(1+x)$. *Right:* $f(x) = \frac{1}{(1+x^2)^{1.8}}$.

where $u_j = u_N(x_j^\lambda)$. Note that the corresponding Lagrange basis function $\{l_j\}_{j=1}^N$ can be expressed as

$$l_j(x) = \sum_{k=0}^{N-1} b_k^j R_k^\lambda(x), \quad \text{with} \quad b_k^j = \frac{R_k^\lambda(x_j^\lambda)\omega_j^\lambda}{\gamma_k^\lambda}, \quad 0 \le j, k \le N-1.$$

Consequently, we can easily derive the associated differential matrix $\mathcal{D}^{L,\alpha,\lambda}$ with Lagrange type bases

$$\mathcal{D}_{i,j}^{L,\alpha,\lambda} = (-\Delta)^{\alpha/2} l_j(x_i^\lambda) = \sum_{k=0}^{N-1} b_k^j (-\Delta)^{\alpha/2} R_j^\lambda(x_i^\lambda), \tag{6.1}$$

where $(-\Delta)^{\alpha/2} R_j^\lambda(x_i^\lambda)$ can be computed via (3.26) and (3.27).

6.2. Numerical examples. We now present several numerical examples to show the performance of the spectral collocation method based on MMGFs. Notice that the collocation method is more practical for problems with variable coefficients and nonlinear problems. Also, we shall carry out comparisons with the Hermite collocation method in [39].

6.2.1. A multiterm fractional model. We first consider the following multiterm fractional Laplacian equation:

$$\sum_{j=1}^{J} \rho_j (-\Delta)^{\alpha_j/2} u(x) = f(x), \quad x \in \mathbb{R}; \quad u(x) \to 0, \ \text{as} \ |x| \to \infty. \tag{6.2}$$

Here we set $J = 4$ and

$$\alpha_1 = 0, \quad \alpha_2 = 0.5 \quad \alpha_3 = 1.5, \quad \alpha_4 = 2,$$
$$\rho_1 = \frac{\pi}{6}, \quad \rho_2 = \frac{\pi}{3}, \quad \rho_3 = \frac{\pi}{3}, \quad \rho_4 = \frac{\pi}{6}.$$

Numerical results with two different souce terms are presented in Figure 5. It can be seen that, similar to the Galerkin methods, the MMGF approach has a much better performance than the Hermite function approach in all cases.

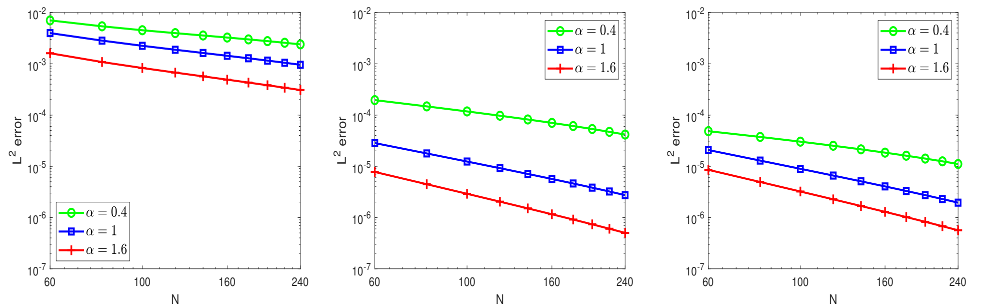

FIG. 6. *Approximation error for* (6.3) *with* $f(x) = \frac{1}{(1+x^2)^{1.2}}$. *Left: Hermite collocation methods in* [39] *with scaling factor* $\mu = 2.5$. *Middle: The MMGF collocation method with* $\lambda = 0$ *and scaling factor* $\mu = 5$. *Right: The MMGF collocation method with* $\lambda = 0.5$ *and scaling factor* $\mu = 5$.

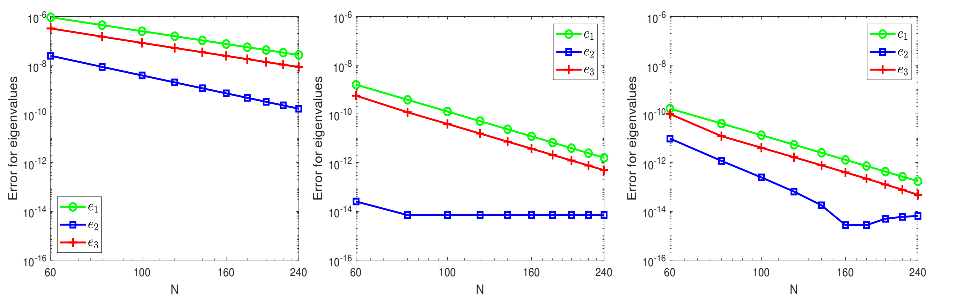

FIG. 7. *Numerical error for the first three eigenvalues of* (6.4). *Left: Generalized Hermite function. Middle: MMGFs with* $\lambda = 0$. *Right: MMGFs with* $\lambda = 0.5$.

6.2.2. Fractional model with variable coefficients. We next consider the following problem:

$$(6.3) \qquad \begin{aligned} &(-\Delta)^{\alpha/2}u(x) + r(x)u(x) = f(x), \quad x \in \mathbb{R}, \\ &u(x) \to 0, \quad \text{as } |x| \to \infty, \end{aligned}$$

where $r(x) = 1 + \exp(-x^2)$ and $f(x) = \frac{1}{(1+x^2)^{1.2}}$. The convergence results for $\alpha = 0.4, 1, 1.6$ are provided in Figure 6 for both approaches. Again, the MMGF spectral collocation method outperforms the Hermite collocation method.

6.2.3. An eigenvalue problem. Finally, we consider the following eigenvalue problem as in [39]:

$$(6.4) \qquad ((-\Delta)^{\alpha/2} + x^2)u(x) = \lambda u(x), \quad x \in \mathbb{R}.$$

Notice that exact eigenvalues for the case of $\alpha = 1$ are available in [25]. For this example, we shall compute the first three eigenvalues by the MMGF spectral collocation method and the Hermite collocation methods for comparison. The numerical results are given in Figure 7, which shows that the MMGF collocation method is more accurate than the Hermite collocation method.

7. Rational spectral methods in multiple dimensions. In this section, we propose the modified rational spectral methods based on a formulation in the Fourier transformed domain in multiple dimensions, and we show that the rational approximation is more accurate than the Hermite approximation (cf. [28]).

To fix the idea, we consider the d-dimensional model problem:

$$\begin{aligned} &(-\Delta)^{\alpha/2}u(x)+\rho u(x)=f(x), \quad x\in\mathbb{R}^d;\\ &u(x)\to 0, \quad \text{as } |x|\to\infty, \end{aligned} \tag{7.1}$$

where $x=(x_1,\ldots,x_d)$ and $|x|=\sqrt{x^tx}$. In the Fourier domain, it takes the form

$$(|\xi|^\alpha+\rho)\hat{u}(\xi)=\hat{f}(\xi), \quad \xi\in\mathbb{R}^d, \tag{7.2}$$

where $\hat{u},\hat{f}$ are the Fourier transform of u, f, respectively. Thus, we have

$$\hat{u}(\xi)=a(\xi)\hat{f}(\xi), \quad a(\xi):=\frac{1}{|\xi|^\alpha+\rho}, \quad \xi\in\mathbb{R}^d. \tag{7.3}$$

This motivates us to construct the spectral scheme in the transformed domain.

Denote

$$\Upsilon_N:=\big\{j=(j_1,\ldots,j_d)\,:\,j_i=0,1,\ldots,N,\ \ 1\le i\le d\big\},$$

and define the tensorial grids and basis functions as

$$x_j^\lambda=(x_{j_1}^\lambda,\ldots,x_{j_d}^\lambda), \quad j\in\Upsilon_N; \quad R_n^\lambda(x)=\prod_{i=1}^d R_{n_i}^\lambda(x_i), \tag{7.4}$$

where $\{x_{j_i}^\lambda\}$ are the one-dimensional grids as in (4.26). We further define the d-dimensional approximation space

$$\mathcal{V}_N^d:=\text{span}\big\{R_n^\lambda : n\in\Upsilon_N\big\}.$$

As the first step, we approximate the source term $f(x)$ by the multidimensional MMGF interpolation,

$$I_N^\lambda f(x)=\sum_{n\in\Upsilon_N}\tilde{f}_n\,R_n^\lambda(x), \tag{7.5}$$

where the coefficients $\{\tilde{f}_n\}_{n\in\Upsilon_N}$ can be computed from the samples $\{f(x_j^\lambda)\}_{j\in\Upsilon_N}$ by the tensorial version of the quadrature (4.27). In particular, if $\lambda=0$, this can be accomplished by the fast Fourier transform. This leads to the approximation

$$\hat{f}(\xi)\approx\widehat{I_N^\lambda f}(\xi)=\sum_{n\in\Upsilon_N}\tilde{f}_n\prod_{i=1}^d\mathscr{F}[R_{n_i}^\lambda](\xi_i), \tag{7.6}$$

where $\mathscr{F}[R_{n_i}^\lambda](\xi_i)$ can be calculated by the formulas in Theorem 7.1 below.

As the second step, we seek the approximation of $\hat{u}(\xi)$ as $\hat{u}_M^N(\xi)\in\mathcal{V}_M^d$ such that

$$\hat{u}_M^N(\xi)=\sum_{m\in\Upsilon_M}\breve{u}_m\,R_m^\lambda(\xi)=\sum_{m\in\Upsilon_M}\breve{u}_m\prod_{i=1}^d R_{m_i}^\lambda(\xi_i), \tag{7.7}$$

where the coefficients are determined by

$$\breve{u}_m=\int_{\mathbb{R}^d}a(\xi)\,\widehat{I_N^\lambda f}(\xi)\,R_m^\lambda(\xi)\,d\xi, \tag{7.8}$$

or by the tensorial quadrature rule based on (4.27),

$$\breve{u}_m = \sum_{j \in \Upsilon_M} a(\xi_j)\, \widehat{I_N^\lambda f}(\xi_j) R_m^\lambda(\xi_j)\, \omega_j^\lambda. \tag{7.9}$$

The last step is to take the Fourier inverse transform of (7.7) leading to the approximation to u as follows:

$$u_M^N(x) = \sum_{m \in \Upsilon_M} \breve{u}_m \prod_{i=1}^{d} \mathscr{F}^{-1}[R_{m_i}^\lambda](x_i). \tag{7.10}$$

Like Theorem 3.4, we have the following formulas for computing the Fourier transform of the basis functions in the above.

THEOREM 7.1. *For real $\lambda > -1/2$, the Fourier transform of the MMGFs can be computed by*

$$\mathscr{F}[R_{2n}^\lambda](\xi) = a_n^\lambda \sum_{k=0}^{n} \frac{(-n)_k (n+\lambda)_k}{(\lambda+\frac{1}{2})_k\, k!} \frac{|\xi|^{k+\lambda/2} K_{k+\lambda/2}(|\xi|)}{2^{k+(\lambda-1)/2}\Gamma(k+(\lambda+1)/2)} \tag{7.11}$$

and

$$\mathscr{F}[R_{2n+1}^\lambda](\xi) = -\mathrm{i}\,\mathrm{sign}(\xi)\, b_n^\lambda \sum_{k=0}^{n} \frac{(-n)_k (n+\lambda+1)_k}{(\lambda+\frac{1}{2})_k k!} \frac{|\xi|^{k+\lambda/2} K_{k+(\lambda-1)/2}(|\xi|)}{2^{k+\lambda/2}\Gamma(k+1+\lambda/2)}, \tag{7.12}$$

where the constants a_n^λ, b_n^λ are defined in (2.18).

Proof. By (3.15), we have that for $\gamma > 0$,

$$\mathscr{F}\Big[\frac{1}{(1+x^2)^\gamma}\Big](\xi) = \frac{2^{1-\gamma}}{\Gamma(\gamma)} |\xi|^{\gamma-\frac{1}{2}} K_{\gamma-\frac{1}{2}}(|\xi|), \quad \xi \in \mathbb{R}.$$

Similarly, we derive from (3.18) that for $\gamma > 1/2$,

$$\mathscr{F}\Big[\frac{x}{(1+x^2)^\gamma}\Big](\xi) = -\mathrm{i}\, \frac{2^{1-\gamma}}{\Gamma(\gamma)}\, \mathrm{sign}(\xi)\, |\xi|^{\gamma-\frac{1}{2}} K_{\gamma-\frac{3}{2}}(|\xi|), \quad \xi \in \mathbb{R}.$$

Consequently, the formulas (7.11)–(7.12) follow from (3.7)–(3.8) directly. ∎

Remark 7.1. In (7.10), we need the inverse transform of $R_n^\lambda(\xi)$, which can be computed by the same formulas (3.7)–(3.8). Indeed, by definition, we have

$$\mathscr{F}^{-1}[R_n^\lambda](x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{\mathrm{i}x\xi} R_n^\lambda(\xi) d\xi = \overline{\mathscr{F}[R_n^\lambda](x)}. \tag{7.13}$$

To conduct the error analysis, we write the scheme (7.7) with (7.8) as

$$u_M^N(x) = \mathscr{F}^{-1}\big[\pi_M^\lambda\big\{a(\xi)\widehat{I_N^\lambda f}(\xi)\big\}\big](x), \tag{7.14}$$

where π_M^λ is the $L^2(\mathbb{R}^d)$ orthogonal projection upon $\mathcal{V}_M^d$. Using the Parseval's identity, we deduce

$$\begin{aligned} \|u_M^N - u\|_{L^2(\mathbb{R}^d)}^2 &= \|\hat{u}_M^N - \hat{u}\|_{L^2(\mathbb{R}^d)}^2 = \|\pi_M^\lambda\{a\widehat{I_N^\lambda f}\} - a\hat{f}\|_{L^2(\mathbb{R}^d)}^2 \\ &\le \big\|\pi_M^\lambda\{a\widehat{I_N^\lambda f} - a\hat{f}\} + \pi_M^\lambda\{a\hat{f}\} - a\hat{f}\big\|_{L^2(\mathbb{R}^d)}^2 \\ &\le \big\|\pi_M^\lambda\{a\widehat{I_N^\lambda f} - a\hat{f}\}\big\|_{L^2(\mathbb{R}^d)}^2 + \big\|\pi_M^\lambda\{a\hat{f}\} - a\hat{f}\big\|_{L^2(\mathbb{R}^d)}^2. \end{aligned} \tag{7.15}$$

We now deal with the first term and find from the L^2-stability of π_M^λ and the Parseval's identity that

$$\begin{aligned}\big\|\pi_M^\lambda\{a\widehat{I_N^\lambda f}-a\hat f\}\big\|^2_{L^2(\mathbb{R}^d)} &\le \big\|a\widehat{I_N^\lambda f}-a\hat f\big\|^2_{L^2(\mathbb{R}^d)} \le c\big\|\widehat{I_N^\lambda f}-\hat f\big\|^2_{L^2(\mathbb{R}^d)}\\ &= c\big\|I_N^\lambda f-f\big\|^2_{L^2(\mathbb{R}^d)}.\end{aligned} \tag{7.16}$$

To derive the error bounds, we resort to the approximation results on the L^2-orthogonal projection and interpolation, which can be derived by following the same argument as in [33] (for $\lambda=0$) and using the one-dimensional results in section 4. For this purpose, we introduce the d-dimensional Sobolev space

$$\mathbb{B}_\lambda^m(\mathbb{R}^d)=\big\{u:\mathscr{D}_x^k u\in L^2_{\varpi^{\lambda+k+1}}(\mathbb{R}^d),\ 0\le |k|_1\le m\big\}, \tag{7.17}$$

where $k=k_1+\cdots+k_d$, and the differential operator and the weight function are

$$\mathscr{D}_x^k u=\mathscr{D}_{x_1}^{k_1}\cdots\mathscr{D}_{x_d}^{k_d}u,\quad \varpi^k(x)=\prod_{j=1}^d(1+x_j^2)^{-k_j}. \tag{7.18}$$

As an extension of (4.9), we denote its seminorm by $|\cdot|_{\mathbb{B}^m(\mathbb{R}^d)}$. Following [33, Thm. 3.1], we can obtain that for $u\in\mathbb{B}_\lambda^m(\mathbb{R}^d)$ with integer $m\ge 0$ and $\lambda>-1/2$, we have

$$\|\pi_M^\lambda u-u\|_{L^2(\mathbb{R}^d)}\le cM^{-m}|u|_{\mathbb{B}_\lambda^m(\mathbb{R}^d)}, \tag{7.19}$$

and for $m\ge d$,

$$\|I_N^\lambda u-u\|_{L^2(\mathbb{R}^d)}\le cN^{-m}|u|_{\mathbb{B}_\lambda^m(\mathbb{R}^d)}. \tag{7.20}$$

Using the above approximation result, we can obtain from (7.15)–(7.16) the error bounds below.

THEOREM 7.2. *Suppose that $a\hat f\in\mathbb{B}_\lambda^m(\mathbb{R}^d)$ and $f\in\mathbb{B}_\lambda^{m'}(\mathbb{R}^d)$ with $m\ge 0$ and $m'\ge d$. Then we have*

$$\|u_M^N-u\|_{L^2(\mathbb{R}^d)}\le cM^{-m}|a\hat f|_{\mathbb{B}_\lambda^m(\mathbb{R}^d)}+cN^{-m'}|f|_{\mathbb{B}_\lambda^{m'}(\mathbb{R}^d)}, \tag{7.21}$$

where c is a positive constant independent of M,N, and f.

Remark 7.2. Note that the scheme (7.7) with (7.9) can be written as

$$u_M^N(x)=\mathscr{F}^{-1}\big[I_M^\lambda\big\{c(\xi)\widehat{I_N^\lambda f}(\xi)\big\}\big](x). \tag{7.22}$$

In fact, we can follow the above lines to perform the analysis with I_M^λ in place of π_M^λ. However, in (7.16), the stability of I_M^λ involves norms with partial derivatives of order d, which should be more involved. Here, we omit the details.

We now consider a two-dimensional example with $f(x,y)=\exp(-\sqrt{x^2+y^2})$. Notice that the Fourier transform of this source term can be computed as

$$\mathscr{F}[f](\xi,\eta)=\frac{1}{(1+\xi^2+\eta^2)^{3/2}}.$$

The corresponding numerical results are presented in Figure 8. Once again, the MMGF collocation method is more accurate and converges faster than the Hermite collocation method.

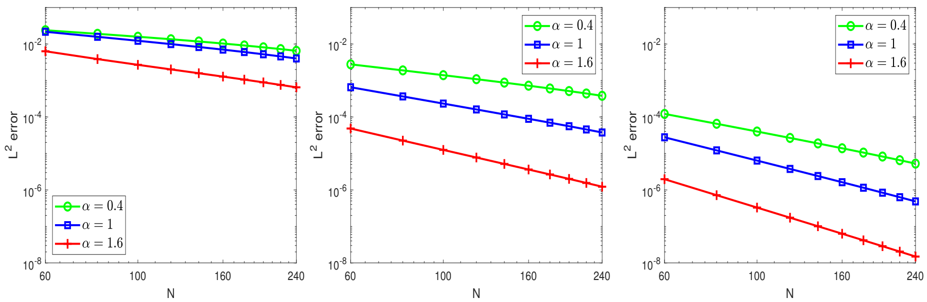

FIG. 8. *Numerical results for the two-dimensional example with* $f(x,y) = \exp(-\sqrt{x^2+y^2})$. *Left: Hermite collocation methods. Middle: MMGF collocation methods with* $\lambda = 0$. *Right: MMGF collocation methods with* $\lambda = 0.5$.

8. Summary and concluding remarks. In this paper, we have developed accurate spectral methods using rational basis (or modified mapped Gegenbauer functions) for PDEs with fractional Laplacian in unbounded domains. The main building block of the spectral algorithms is some explicit formulas for the Fourier transforms and fractional Laplacian of the rational basis. With these, we can construct rational spectral-Galerkin and collocation schemes by precomputing the associated fractional differentiation matrices. We obtain optimal error estimates of rational spectral approximation in the fractional Sobolev spaces and analyze the optimal convergence of the proposed Galerkin scheme. Numerical results show that the rational method outperforms the Hermite function approach. Future studies along this line will include the error estimates of the rational collocation methods in section 6, fast preconditioner/solvers for high dimensional problems, and applications of the MMGF approach to tempered fractional PDEs.

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