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NONTENSORIAL GENERALISED HERMITE SPECTRAL METHODS FOR PDES WITH FRACTIONAL LAPLACIAN AND SCHRÖDINGER OPERATORS

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Abstract. In this paper, we introduce two families of nontensorial generalised Hermite polynomials/functions (GHPs/GHFs) in arbitrary dimensions, and develop efficient and accurate spectral methods for solving PDEs with integral fractional Laplacian (IFL) and/or Schrödinger operators in $\mathbb{R}^d$. As a generalisation of the G. Szegö's family in 1D (1939), the first family of multivariate GHPs (resp. GHFs) are orthogonal with respect to the weight function $|\boldsymbol{x}|^{2\mu}\mathrm{e}^{-|\boldsymbol{x}|^2}$ (resp. $|\boldsymbol{x}|^{2\mu}$) in $\mathbb{R}^d$. We further construct the adjoint generalised Hermite functions (A-GHFs), which have an interwoven connection with the corresponding GHFs through the Fourier transform, and are orthogonal with respect to the inner product $[u,v]_{H^s(\mathbb{R}^d)} = ((-\Delta)^{s/2}u, (-\Delta)^{s/2}v)_{\mathbb{R}^d}$ associated with the IFL of order $s > 0$. As an immediate consequence, the spectral-Galerkin method using A-GHFs as basis functions leads to a diagonal stiffness matrix for the IFL (which is known to be notoriously difficult and expensive to discretise). The new basis also finds remarkably efficient in solving PDEs with the fractional Schrödinger operator: $(-\Delta)^s + |\boldsymbol{x}|^{2\mu}$ with $s \in (0,1]$ and $\mu > -1/2$ in $\mathbb{R}^d$. We construct the second family of multivariate nontensorial Müntz-type GHFs, which are orthogonal with respect to an inner product associated with the underlying Schrödinger operator, and are tailored to the singularity of the solution at the origin. We demonstrate that the Müntz-type GHF spectral method leads to sparse matrices and spectrally accurate solution to some Schrödinger eigenvalue problems.

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1. Introduction

In the seminal monograph ([43], p. 371) (1939), Szegö introduced for the first time a generalisation of the Hermite polynomials (denoted by $H_n^{(\mu)}(x)$, $\mu > -1/2$, $x \in \mathbb{R} := (-\infty, \infty)$ and dubbed as generalised Hermite

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polynomials (GHPs)), through a second-order differential equation in an exercise problem. The GHPs are orthogonal with respect to the weight function $|x|^{2\mu}\mathrm{e}^{-x^2}$ in $\mathbb{R}$. Chihara was among the first who systematically studied the properties of the GHPs, and the associated generalised Hermite functions (GHFs): $\widehat{H}_n^{(\mu)}(x) := \mathrm{e}^{-x^2/2}H_n^{(\mu)}(x)$ (orthogonal with respect to the weight function $|x|^{2\mu}$ in $\mathbb{R}$) in his PhD thesis [10] entitled as "Generalised Hermite Polynomials" (1955). Later, some standard properties were collected in his book [11] (1978). Whereas the usual Hermite polynomials/functions are well-studied especially in spectral approximations, there have been very limited works on this generalised family (see, *e.g.,* [30, 35–37] for the properties or further generalisations). In particular, the generalised Hermite spectral method in terms of algorithms, analysis and applications are still under-explored, which is indeed a topic worthy of investigation.

The main purpose of this paper is to construct two families of nontensorial GHPs/GHFs in arbitrary dimensions, and explore their applications in solving PDEs with the IFL and/or Schrödinger operators.

Firstly, we construct the d-dimensional GHPs $\{H_{k,\ell}^{\mu,n}(\boldsymbol{x})\}$ (*cf.* (2.12)) and GHFs $\{\widehat{H}_{k,\ell}^{\mu,n}(\boldsymbol{x})\}$ (*cf.* (2.13)), which are orthogonal with respect to the weight functions $|\boldsymbol{x}|^{2\mu}\mathrm{e}^{-|\boldsymbol{x}|^2}$ and $|\boldsymbol{x}|^{2\mu}$ in $\mathbb{R}^d$ with $\mu > -\frac{1}{2}$, respectively. In one dimension, they reduce to Szegö's GHPs/GHFs (up to a constant multiple). More importantly, we further introduce a family of adjoint generalised Hermite functions (A-GHFs) $\{\check{H}_{k,\ell}^{\mu,n}(\boldsymbol{x})\}$ (*cf.* (2.25)) and derive some appealing properties that are essential for developing fast and accurate spectral algorithms. We show that the adjoint pair is closely interwoven through the Fourier transform

$$\mathscr{F}[\widehat{H}_{k,\ell}^{\mu,n}](\boldsymbol{\xi}) = \mathrm{i}^{n+2k}\check{H}_{k,\ell}^{\mu,n}(\boldsymbol{\xi}), \quad \mathscr{F}[\check{H}_{k,\ell}^{\mu,n}](\boldsymbol{\xi}) = (-\mathrm{i})^{n+2k}\widehat{H}_{k,\ell}^{\mu,n}(\boldsymbol{\xi}). \tag{1.1}$$

Notably, by construction, the A-GHFs are orthogonal with respect to the inner product that induces the so-called Gagliardo semi-norm of the fractional Sobolev space $H^s(\mathbb{R}^d)$ for $s \in (0,1]$, that is,

$$[\check{H}_{k,\ell}^{s,n}, \check{H}_{j,\iota}^{s,m}]_{H^s(\mathbb{R}^d)} = \big((-\Delta)^{\frac{s}{2}}\check{H}_{k,\ell}^{s,n}, (-\Delta)^{\frac{s}{2}}\check{H}_{j,\iota}^{s,m}\big)_{\mathbb{R}^d} = \delta_{jk}\delta_{mn}\delta_{\ell\iota}, \tag{1.2}$$

where $(-\Delta)^s$ is the integral fractional Laplacian operator (*cf.* (2.28) and (2.29)). An immediate implication is that the use of A-GHFs as basis functions in the spectral-Galerkin approximation of the IFL leads to a diagonal stiffness matrix. In contrast, it has been a nightmare for computing this matrix in a usual tensorial Hermite spectral method when $d = 3$ (*cf.* [29]). Moreover, this new basis offers efficient spectral algorithm for solving PDEs with the fractional Schrödinger operator: $(-\Delta)^s + V(\boldsymbol{x})$ with $V(\boldsymbol{x}) = |\boldsymbol{x}|^{2\mu}$ or more general $V(\boldsymbol{x}) = |\boldsymbol{x}|^{2\mu}W(\boldsymbol{x})$ (where W is smooth function of Schwartz class) with $s \in (0,1]$ and $\mu > -1/2$. In light of the orthogonality (1.2), the stiffness matrix under the Galerkin framework using the basis $\{\check{H}_{k,\ell}^{s,n}\}$ becomes diagonal, while the singular potential $|\boldsymbol{x}|^{2\mu}$ can be treated as the weight function, since $\check{H}_{k,\ell}^{s,n}$ can be represented as a linear combination of $\{\widehat{H}_{j,l}^{\mu,n}\}$ (*cf.* (2.20) and (2.25)). Indeed, the A-GHFs can provide a viable tool for the solutions of fractional Schrödinger problems (see, *e.g.,* [5, 6, 22, 47]).

It is noteworthy that the 3D GHPs (with $\mu = 0$ and an appropriate scaling) reduce to the Burnett polynomials [8] (1936), which are mutually orthogonal with respect to the Maxwellian $\mathcal{M}(\boldsymbol{x}) = (2\pi)^{-3/2}\mathrm{e}^{-|\boldsymbol{x}|^2/2}$, and have proven to be a useful basis in solving kinetic equations (*cf.* [9, 20] and the references therein). It is important to point out that the GHFs with $\mu = 0$ are eigenfunctions of the harmonic oscillator (*cf.* (2.23)):

$$\big(-\Delta + |\boldsymbol{x}|^2\big)\widehat{H}_{k,\ell}^{0,n}(\boldsymbol{x}) = (4k + 2n + d)\widehat{H}_{k,\ell}^{0,n}(\boldsymbol{x}). \tag{1.3}$$

In fact, such an attractive property (in 2D) has been explored in [4] for computing the ground states and dynamics of the Bose-Einstein condensation.

It is of fundamental and practical interest to search for the explicit eigen-functions of the Schrödinger operator with a more general potential or some variance of the operator in (1.3), which is the second purpose of this paper. The main finding (*cf.* Thm. 4.2) is that for $\theta > \max(1-d/2, 0)$, there exists a family of Müntz-type GHFs $\{\widehat{\mathcal{H}}_{k,\ell}^{\theta,n}\}$ (*cf.* (4.3)) satisfying

$$\big(-\Delta + \theta^2|\boldsymbol{x}|^{4\theta-2}\big)\widehat{\mathcal{H}}_{k,\ell}^{\theta,n}(\boldsymbol{x}) = 2\theta^2\big((n + d/2 - 1)/\theta + 2k + 1\big)\,|\boldsymbol{x}|^{2\theta-2}\widehat{\mathcal{H}}_{k,\ell}^{\theta,n}(\boldsymbol{x}). \tag{1.4}$$

TABLE 1. Two families of GHPs/GHFs and their essential properties.

	Type	Property
Generalised Hermite polynomials & functions	d-D GHP: $H^{\mu,n}_{k,\ell}(\boldsymbol{x})$ in (2.12) 1D GHP: $H^{(\mu)}_n(x)$ in [43]	Orthogonal w.r.t. $\lvert\boldsymbol{x}\rvert^{2\mu}\mathrm{e}^{-\lvert\boldsymbol{x}\rvert^2}$; Burnett polynomials [8], if $\mu=0$
	d-D GHF: $\widehat{H}^{\mu,n}_{k,\ell}(\boldsymbol{x})$ in (2.13) 1D GHF: $\widehat{H}^{(\mu)}_n(x)$ in (2.42)	Orthogonal w.r.t. $\lvert\boldsymbol{x}\rvert^{2\mu}$; Eigenfunctions of $-\Delta+\lvert\boldsymbol{x}\rvert^2$, if $\mu=0$
	d-D A-GHF: $\breve{H}^{\mu,n}_{k,\ell}(\boldsymbol{x})$ in (2.25) 1D A-GHF: $\breve{H}^{(\mu)}_n(x)$ in (2.46)	Orthogonal w.r.t.$((-\Delta)^{\frac{\mu}{2}}\cdot,(-\Delta)^{\frac{\mu}{2}}\cdot)_{\mathbb{R}^d}$; Diagonal stiffness matrix for $(-\Delta)^{\mu}$, if $\mu>0$
Müntz-type generalised	d-D M-GHF: $\widehat{\mathcal{H}}^{\theta,n}_{k,\ell}(\boldsymbol{x})$ in (4.3)	Orthogonal w.r.t. $(\nabla\cdot,\nabla\cdot)_{\mathbb{R}^d}+\theta^2(\lvert\boldsymbol{x}\rvert^{4\theta-2}\cdot,\cdot)_{\mathbb{R}^d}$
Hermite functions	$\widehat{\mathcal{H}}^{\frac12,n}_{k,\ell}(\boldsymbol{x})$ in Subsection 4.2	Eigenfunctions (with a scaling) of $-\frac12\Delta+\frac{\lvert Z\rvert}{\lvert\boldsymbol{x}\rvert}$
	$\widehat{\mathcal{H}}^{\frac{1}{\mu+1},n}_{k,\ell}(\boldsymbol{x})$ in Subsection 4.3	Optimal basis for the Schrödinger operator: $-\frac12\Delta+\lvert Z\rvert\lvert\boldsymbol{x}\rvert^{\frac{2\nu-2\mu}{\mu+1}}$ for μ,ν in (4.16)

In particular, for $\theta=1/2$, we find

$$\Big(-\Delta-\frac{n+k+(d-1)/2}{\lvert\boldsymbol{x}\rvert}\Big)\widehat{\mathcal{H}}^{\frac12,n}_{k,\ell}(\boldsymbol{x})=-\frac14\widehat{\mathcal{H}}^{\frac12,n}_{k,\ell}(\boldsymbol{x}). \tag{1.5}$$

With a proper scaling, this gives the eigen-pairs of the Schrödinger operator with the Coulomb potential: $-\frac12\Delta-\frac{\lvert Z\rvert}{\lvert\boldsymbol{x}\rvert}$, where Z is a nonzero constant (*cf.* Cor. 4.3). By construction, this new family $\{\widehat{\mathcal{H}}^{\theta,n}_{k,\ell}\}$ in the radial direction turns out to be some special Müntz functions, so it is dubbed as Müntz-type for distinction. We remark that a Müntz polynomial $\sum_{k=0}^{n}a_kr^{\lambda_k}$ is generated by a Müntz sequence: $\lambda_0<\lambda_1<\lambda_2<\cdots<\lambda_n$ (*cf.* [31] (1914)), and the set of Müntz polynomials with $\lambda_0=0$, and real coefficients $\{a_k\}$ are dense in the space of continuous functions if and only if $\sum_{k=0}^{\infty}\lambda_k^{-1}=\infty$ (*cf.* [7] and the references therein). Such a tool finds very effective in approximating singular solutions (see, *e.g.,* [19,39]). We shall demonstrate in Section 4 that the Müntz-type GHF spectral-Galerkin approach is the method of choice of the Schrödinger eigenvalue problems with the fractional power potential in terms of both the efficiency and accuracy. In particular, the spectral accuracy can be achieved by using such basis function to match the singular behaviours of the eigenfunctions.

In Table 1, we provide a roadmap of two types of generalisations and some of their properties that are essential for developing efficient spectral algorithms for PDEs with integral fractional Laplacian in Section 2 and the Schrödinger eigenvalue problems in Section 4. In Subsection 2.4, we highlight the differences and connections with the relevant existing generalisations, and further testify that most of our constructions herein are new.

2. Multivariate nontensorial generalised Hermite polynomials/functions

In this section, we first make necessary preparations by introducing some notation and properties of the spherical harmonic functions. We then define the GHPs and GHFs upon the generalised Laguerre polynomials and spherical harmonics, and further construct a family of adjoint GHFs. We present various appealing properties of these basis functions, which are essential for the efficient spectral algorithms to be developed in the forthcoming section. We conclude this section by elaborating on their differences and connections with the most relevant Hermite-related polynomials/functions in literature.

2.1. Preliminaries

Let $\mathbb{R} = (-\infty, \infty)$, $\mathbb{N} = \{1, 2, \cdots\}$, and $\mathbb{N}_0 := \{0\} \cup \mathbb{N}$. For $d \in \mathbb{N}$, we denote by $\mathbb{R}^d$ the d-dimensional Euclidean space with the inner product and norm $\langle \boldsymbol{x}, \boldsymbol{y} \rangle := \sum_{i=1}^d x_i y_i$, and $r = |\boldsymbol{x}| := \sqrt{\langle \boldsymbol{x}, \boldsymbol{x} \rangle}$, respectively, for any $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d$. Denote the unit vector along any nonzero vector $\boldsymbol{x}$ by $\hat{\boldsymbol{x}} = \boldsymbol{x}/|\boldsymbol{x}|$. Recall the d-dimensional spherical coordinates

$$\begin{aligned} &x_1 = r\cos\theta_1;\ x_2 = r\sin\theta_1\cos\theta_2;\ \cdots\cdots;\ x_{d-1} = r\sin\theta_1\cdots\sin\theta_{d-2}\cos\theta_{d-1};\\ &x_d = r\sin\theta_1\cdots\sin\theta_{d-2}\sin\theta_{d-1}, \quad \theta_1,\cdots,\theta_{d-2} \in [0,\pi], \quad \theta_{d-1} \in [0, 2\pi], \end{aligned} \tag{2.1}$$

with the spherical volume element

$$\mathrm{d}\boldsymbol{x} = r^{d-1}\sin^{d-2}(\theta_1)\sin^{d-3}(\theta_2)\cdots\sin(\theta_{d-2})\,\mathrm{d}r\,\mathrm{d}\theta_1\,\mathrm{d}\theta_2\cdots\mathrm{d}\theta_{d-1} := r^{d-1}\mathrm{d}r\,\mathrm{d}\sigma(\hat{\boldsymbol{x}}). \tag{2.2}$$

In spherical coordinates, the d-dimensional Laplacian takes the form

$$\Delta = \partial_r^2 + \frac{d-1}{r}\partial_r + \frac{1}{r^2}\Delta_{\mathbb{S}^{d-1}}, \tag{2.3}$$

where $\Delta_{\mathbb{S}^{d-1}}$ is the Laplace-Beltrami operator on the unit sphere $\mathbb{S}^{d-1} := \{\boldsymbol{x} \in \mathbb{R}^d : |\boldsymbol{x}| = 1\}$. Define the inner product of $L^2(\mathbb{S}^{d-1})$ as

$$\langle f, g \rangle_{\mathbb{S}^{d-1}} := \int_{\mathbb{S}^{d-1}} f(\hat{\boldsymbol{x}})g(\hat{\boldsymbol{x}})\,\mathrm{d}\sigma(\hat{\boldsymbol{x}}).$$

We next introduce the d-dimensional spherical harmonics as in [12]. Let $\mathcal{P}_n^d$ be the space of all real d-dimensional homogeneous polynomials of degree n as follows

$$\mathcal{P}_n^d = \mathrm{span}\big\{\boldsymbol{x}^{\boldsymbol{k}} = x_1^{k_1}x_2^{k_2}\ldots x_d^{k_d} : k_1 + k_2 + \cdots + k_d = n\big\}. \tag{2.4}$$

As an important subspace of $\mathcal{P}_n^d$, the space of all real harmonic polynomials of degree n is defined as

$$\mathcal{H}_n^d := \big\{P \in \mathcal{P}_n^d : \Delta P(\boldsymbol{x}) = 0\big\}. \tag{2.5}$$

It is known that the dimensionality

$$\dim(\mathcal{P}_n^d) = \binom{n+d-1}{n}, \quad \dim(\mathcal{H}_n^d) = \binom{n+d-1}{n} - \binom{n+d-3}{n-2} := a_n^d, \tag{2.6}$$

where it is understood that for $n = 0, 1$, the value of the second binomial coefficient is zero (*cf.* [12] (1.1.5)). In fact, for $d = 1$, all harmonic polynomials are spanned by $\{1, x\}$.

The d-dimensional spherical harmonics are the restrictions of harmonic polynomials in $\mathcal{H}_n^d$ to $\mathbb{S}^{d-1}$, denoted by $\mathcal{H}_n^d\big|_{\mathbb{S}^{d-1}}$. It is important to remark the correspondence between a harmonic polynomial and the related spherical harmonic function (*cf.* [12], Ch. 1): for any $Y(\boldsymbol{x}) \in \mathcal{H}_n^d$,

$$Y(\boldsymbol{x}) = |\boldsymbol{x}|^n Y(\boldsymbol{x}/|\boldsymbol{x}|) = r^n Y(\hat{\boldsymbol{x}}), \tag{2.7}$$

with $Y(\hat{\boldsymbol{x}}) \in \mathcal{H}_n^d\big|_{\mathbb{S}^{d-1}}$. It is noteworthy that $Y(\boldsymbol{x})$ is a homogeneous polynomial in $\mathbb{R}^d$, while $Y(\hat{\boldsymbol{x}})$ is a non-polynomial function on the unit sphere. For $n \in \mathbb{N}_0$, let $\{Y_\ell^n : 1 \leqslant \ell \leqslant a_n^d\}$ be the real (orthogonal) spherical harmonic basis of $\mathcal{H}_n^d|_{\mathbb{S}^{d-1}}$, and note that the spherical harmonics of different degree are mutually orthogonal (*cf.* [12], Thm. 1.1.2), *i.e.*, $\mathcal{H}_n^d|_{\mathbb{S}^{d-1}} \perp \mathcal{H}_m^d|_{\mathbb{S}^{d-1}}$ for $m \neq n$. Thus, we have

$$\langle Y_\ell^n, Y_\iota^m \rangle_{\mathbb{S}^{d-1}} = \int_{\mathbb{S}^{d-1}} Y_\ell^n(\hat{\boldsymbol{x}})Y_\iota^m(\hat{\boldsymbol{x}})\,\mathrm{d}\sigma(\hat{\boldsymbol{x}}) = \delta_{nm}\delta_{\ell\iota}, \quad (\ell, n), (\iota, m) \in \Upsilon_\infty^d, \tag{2.8}$$

where we introduce two-related the index sets

$$\begin{aligned}\Upsilon_\infty^d &= \big\{(\ell,n) : 1 \leqslant \ell \leqslant a_n^d,\ \ 0 \leqslant n < \infty,\ \ \ell, n \in \mathbb{N}_0\big\},\\ \Upsilon_N^d &= \big\{(\ell,n) : 1 \leqslant \ell \leqslant a_n^d,\ \ 0 \leqslant n \leqslant N,\ \ \ell, n \in \mathbb{N}_0\big\}.\end{aligned} \tag{2.9}$$

The spherical harmonic basis functions are eigenfunctions of the Laplace-Beltrami problem

$$\Delta_{\mathbb{S}^{d-1}} Y_\ell^n(\hat{\boldsymbol{x}}) = -n(n+d-2) Y_\ell^n(\hat{\boldsymbol{x}}). \tag{2.10}$$

The second building block of the GHPs/GHFs is the generalized Laguerre polynomials, denoted by $L_k^{(\alpha)}(z)$ for $z \in (0,\infty)$ and $\alpha > -1$. They are orthogonal with respect to the weight function $z^\alpha \mathrm{e}^{-z}$, that is,

$$\int_0^\infty L_k^{(\alpha)}(z) L_j^{(\alpha)}(z)\, z^\alpha\, \mathrm{e}^{-z}\, \mathrm{d}z = \frac{\Gamma(k+\alpha+1)}{k!}\delta_{kj}, \quad k, j \in \mathbb{N}_0, \tag{2.11}$$

where we refer to [43], ([25], Ch. 4) and ([38], Ch. 7) for more properties.

2.2. Generalized Hermite polynomials/functions in $\mathbb{R}^{\boldsymbol{d}}$

Definition 2.1. For $\mu > -\frac{1}{2}$, $k \in \mathbb{N}_0$ and $(\ell,n) \in \Upsilon_\infty^d$, we define the d-dimensional generalised Hermite polynomials as

$$\begin{aligned} H_{k,\ell}^{\mu,n}(\boldsymbol{x}) := H_{k,\ell}^{\mu,n}(\boldsymbol{x}; d) &= L_k^{(n+\frac{d-2}{2}+\mu)}(|\boldsymbol{x}|^2) Y_\ell^n(\boldsymbol{x}) \\ &= r^n L_k^{(n+\frac{d-2}{2}+\mu)}(r^2) Y_\ell^n(\hat{\boldsymbol{x}}), \quad \boldsymbol{x} = r\,\hat{\boldsymbol{x}}, \end{aligned} \tag{2.12}$$

and the d-dimensional generalised Hermite functions as

$$\widehat{H}_{k,\ell}^{\mu,n}(\boldsymbol{x}) = \sqrt{1/\gamma_{k,n}^{\mu,d}}\, \mathrm{e}^{-\frac{|\boldsymbol{x}|^2}{2}} H_{k,\ell}^{\mu,n}(\boldsymbol{x}), \quad \text{where} \quad \gamma_{k,n}^{\mu,d} := \frac{\Gamma(k+n+\frac{d}{2}+\mu)}{2\,k!}. \tag{2.13}$$

Remark 2.2. As we shall see later, the one-dimensional GHPs (up to a constant multiple) coincide with the one-dimensional generalisation first introduced in Szegö ([43], p. 371) (1939), after which we name the above new families. Indeed, they include several special types of multivariate Hermite polynomials/functions with many applications in both theory and numerics. For example, the three-dimensional GHPs with $\mu = 0$ and a proper scaling lead to the Burnett polynomials [8] (1936) which have rich applications in kinetic theory (see [9] and the references therein). The notion of constructing special Laguerre-Fourier basis functions (relevant to the two-dimensional GHPs with $\mu = 0$) for computing the ground states and dynamics of Bose-Einstein condensation [34] was found effective in *e.g.,* [4]. □

Before we consider the applications of GHPs and GHFs, we first present some attractive properties. By construction, they enjoy the following important orthogonality.

Theorem 2.3. *For $\mu > -\frac{1}{2}$, $k, j \in \mathbb{N}_0$ and $(\ell,n), (\iota, m) \in \Upsilon_\infty^d$, the GHPs are mutually orthogonal with respect to the weight function $|\boldsymbol{x}|^{2\mu}\mathrm{e}^{-|\boldsymbol{x}|^2}$, namely,*

$$\int_{\mathbb{R}^d} H_{k,\ell}^{\mu,n}(\boldsymbol{x}) H_{j,\iota}^{\mu,m}(\boldsymbol{x})\, |\boldsymbol{x}|^{2\mu}\, \mathrm{e}^{-|\boldsymbol{x}|^2}\, \mathrm{d}\boldsymbol{x} = \gamma_{k,n}^{\mu,d}\, \delta_{mn}\delta_{kj}\delta_{\ell\iota}, \tag{2.14}$$

and the GHFs are orthonormal, viz.,

$$\int_{\mathbb{R}^d} \widehat{H}_{k,\ell}^{\mu,n}(\boldsymbol{x}) \widehat{H}_{j,\iota}^{\mu,m}(\boldsymbol{x})\, |\boldsymbol{x}|^{2\mu}\, \mathrm{d}\boldsymbol{x} = \delta_{mn}\delta_{kj}\delta_{\ell\iota}. \tag{2.15}$$

Proof. The orthogonality (2.15) is a direct consequence of (2.13) and (2.14), so we only need to show (2.14). In view of the definition (2.12), we use the spherical coordinates transformation (2.1)–(2.2), and find from the orthogonality (2.8) and (2.11) that

$$
\begin{aligned}
&\int_{\mathbb{R}^d} H_{k,\ell}^{\mu,n}(\boldsymbol{x}) H_{j,\iota}^{\mu,m}(\boldsymbol{x})\, |\boldsymbol{x}|^{2\mu}\, \mathrm{e}^{-|\boldsymbol{x}|^2}\, \mathrm{d}\boldsymbol{x} \\
&= \int_0^\infty L_k^{(n+\frac{d-2}{2}+\mu)}(r^2)\, L_j^{(m+\frac{d-2}{2}+\mu)}(r^2)\, r^{2\mu+2n+d-1} \mathrm{e}^{-r^2}\, \mathrm{d}r \int_{\mathbb{S}^{d-1}} Y_\ell^n(\hat{\boldsymbol{x}}) Y_\iota^m(\hat{\boldsymbol{x}})\, \mathrm{d}\sigma(\hat{\boldsymbol{x}}) \\
&= \delta_{mn}\delta_{\ell\iota} \int_0^\infty L_k^{(n+\frac{d-2}{2}+\mu)}(r^2)\, L_j^{(m+\frac{d-2}{2}+\mu)}(r^2)\, r^{2\mu+2n+d-1} \mathrm{e}^{-r^2}\, \mathrm{d}r \\
&= \frac{1}{2}\delta_{mn}\delta_{\ell\iota} \int_0^\infty L_k^{(n+\frac{d-2}{2}+\mu)}(\rho)\, L_j^{(n+\frac{d-2}{2}+\mu)}(\rho)\, \rho^{n+\frac{d-2}{2}+\mu} \mathrm{e}^{-\rho}\, \mathrm{d}\rho \\
&= \frac{\Gamma(k+n+\frac{d}{2}+\mu)}{2k!} \delta_{mn}\delta_{kj}\delta_{\ell\iota} = \gamma_{k,n}^{\mu,d}\, \delta_{mn}\delta_{kj}\delta_{\ell\iota},
\end{aligned}
$$

which yields (2.14) and ends the proof. □

The d-dimensional GHPs/GHFs satisfy the recurrence relations.

Proposition 2.4. *For $\mu > -\frac{1}{2}$ and fixed $(\ell, n) \in \Upsilon_\infty^d$, we have the following recurrence relations in k:*

$$
(k+1)H_{k+1,\ell}^{\mu,n}(\boldsymbol{x}) = \big(2k+n+\frac{d}{2}+\mu-|\boldsymbol{x}|^2\big)H_{k,\ell}^{\mu,n}(\boldsymbol{x}) - \big(k+n+\frac{d}{2}-1+\mu\big)H_{k-1,\ell}^{\mu,n}(\boldsymbol{x}), \tag{2.16}
$$

and for the GHFs,

$$
a_k\, \widehat{H}_{k+1,\ell}^{\mu,n}(\boldsymbol{x}) = (b_k - |\boldsymbol{x}|^2)\widehat{H}_{k,\ell}^{\mu,n}(\boldsymbol{x}) - c_k \widehat{H}_{k-1,\ell}^{\mu,n}(\boldsymbol{x}), \tag{2.17}
$$

where

$$
a_k = \sqrt{(k+1)(k+n+d/2+\mu)}, \quad b_k = 2k+n+d/2+\mu, \quad c_k = \sqrt{k(k-1+n+d/2+\mu)}.
$$

Proof. Recall the three-term recurrence relation of the Laguerre polynomials (*cf.* [43]):

$$
(k+1)L_{k+1}^{(\alpha)}(z) = (2k+\alpha+1-z)L_k^{(\alpha)}(z) - (k+\alpha)L_{k-1}^{(\alpha)}(z). \tag{2.18}
$$

Then the relation (2.16) is a direct consequence of (2.12) and (2.18). From (2.13), we have

$$
H_{k,\ell}^{\mu,n}(\boldsymbol{x}) = \sqrt{\gamma_{k,n}^{\mu,d}}\, \mathrm{e}^{\frac{|\boldsymbol{x}|^2}{2}}\, \widehat{H}_{k,\ell}^{\mu,n}(\boldsymbol{x}), \tag{2.19}
$$

so substituting it into (2.16) and working out the constants, we obtain (2.17). □

The GHFs with different parameters are connected through the following identity, which finds very useful in the algorithm development.

Proposition 2.5. *For $\mu, \nu > -\frac{1}{2}$ and $(\ell, n) \in \Upsilon_\infty^d$, there holds*

$$
\widehat{H}_{k,\ell}^{\mu,n}(\boldsymbol{x}) = \sum_{j=0}^{k} {}_{\nu}^{\mu}\mathbb{C}_j^k\, \widehat{H}_{j,\ell}^{\nu,n}(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^d, \quad k \in \mathbb{N}_0, \tag{2.20}
$$

where the connection coefficients are given by

$$
{}_{\nu}^{\mu}\mathbb{C}_j^k = \frac{\Gamma(k-j+\mu-\nu)}{\Gamma(\mu-\nu)\,(k-j)!} \sqrt{\frac{k!\,\Gamma(j+n+\frac{d}{2}+\nu)}{j!\,\Gamma(k+n+\frac{d}{2}+\mu)}}. \tag{2.21}
$$

Proof. Recall the property of the generalized Laguerre polynomials (*cf.* [3] (7.4)):

$$L_k^{(\mu+\beta+1)}(z) = \sum_{j=0}^{k} \frac{\Gamma(k-j+\beta+1)}{\Gamma(\beta+1)(k-j)!} L_j^{(\mu)}(z), \tag{2.22}$$

so we can derive the identity from Definition 2.1 and direct calculation. □

Remark 2.6. As $\Gamma(0)=\infty$, we can find that in the limiting sense: ${}^{\mu}_{\mu}\mathbb{C}^k_j = \delta_{kj}$. □

Remarkably, for $\mu=0$, the GHFs are the eigenfunctions of the harmonic oscillator: $-\Delta+|\boldsymbol{x}|^2$, are essential for the error analysis to be conducted in the forthcoming section.

Lemma 2.7. *For $k\in\mathbb{N}_0, (\ell,n)\in\Upsilon^d_\infty$, the GHFs with $\mu=0$ satisfy*

$$\big(-\Delta+|\boldsymbol{x}|^2\big)\widehat{H}^{0,n}_{k,\ell}(\boldsymbol{x}) = (4k+2n+d)\,\widehat{H}^{0,n}_{k,\ell}(\boldsymbol{x}). \tag{2.23}$$

Proof. According to Lemma 2.1 of [28] with $\alpha=n+d/2-1$ and $\beta=\alpha+1-d/2$, we have

$$\Big[\partial_r^2+\frac{d-1}{r}\partial_r-\frac{n(n+d-2)}{r^2}-r^2+4k+2n+d\Big]\Big[r^n L_k^{(n+d/2-1)}(r^2)\,\mathrm{e}^{-\frac{r^2}{2}}\Big]=0. \tag{2.24}$$

In view of $Y(\boldsymbol{x})=r^nY(\hat{\boldsymbol{x}})$, we obtain from (2.3), (2.10), (2.12), (2.13) and (2.24) that

$$\begin{aligned}
-\Delta\widehat{H}^{0,n}_{k,\ell}(\boldsymbol{x}) &= -\sqrt{1/\gamma^{0,d}_{k,n}}\Big[\partial_r^2+\frac{d-1}{r}\partial_r-\frac{n(n+d-2)}{r^2}\Big]\Big[r^n\,L_k^{(n+d/2-1)}(r^2)\,\mathrm{e}^{-\frac{r^2}{2}}\Big]\,Y(\hat{\boldsymbol{x}})\\
&= \sqrt{1/\gamma^{0,d}_{k,n}}\big[-r^2+4k+2n+d\big]\Big[r^nL_k^{(n+d/2-1)}(r^2)\,\mathrm{e}^{-\frac{r^2}{2}}\Big]\,Y(\hat{\boldsymbol{x}})\\
&= (-r^2+4k+2n+d)\widehat{H}^{0,n}_{k,\ell}(\boldsymbol{x}),
\end{aligned}$$

which leads to (2.23). □

2.3. Adjoint generalized Hermite functions in $\mathbb{R}^{\boldsymbol{d}}$

Definition 2.8. For $\mu>-\frac{1}{2}$ and $(\ell,n)\in\Upsilon^d_\infty$, the d-dimensional adjoint GHFs are defined by

$$\breve{H}^{\mu,n}_{k,\ell}(\boldsymbol{x}) = \sum_{j=0}^{k}(-1)^{k-j}\,{}^{\mu}_{0}\mathbb{C}^k_j\,\widehat{H}^{0,n}_{j,\ell}(\boldsymbol{x}),\quad \boldsymbol{x}\in\mathbb{R}^d,\ \ k\in\mathbb{N}_0, \tag{2.25}$$

where the coefficients $\{{}^{\mu}_{0}\mathbb{C}^k_j\}$ are given by (2.21).

Remark 2.9. In light of the connection relation in Proposition 2.5, it is evident that $\breve{H}^{\mu,n}_{k,\ell}(\boldsymbol{x})$ can be expressed as a linear combination of the counterparts $\big\{\widehat{H}^{\mu,n}_{j,\ell}(\boldsymbol{x})\big\}_{j=0}^{k}$. □

It is seen from (2.20) (with $\nu=0$) that the GHF can be represented as

$$\widehat{H}^{\mu,n}_{k,\ell}(\boldsymbol{x}) = \sum_{j=0}^{k}{}^{\mu}_{0}\mathbb{C}^k_j\,\widehat{H}^{0,n}_{j,\ell}(\boldsymbol{x}), \tag{2.26}$$

which differs from its adjoint in (2.25) by the sign of the coefficients. Notably, such a subtlety results in an intimate relation between this adjoint pair through the Fourier transform:

$$\hat{u}(\boldsymbol{\xi}) := \mathscr{F}[u](\boldsymbol{\xi}) = \frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d}u(\boldsymbol{x})\,\mathrm{e}^{-\mathrm{i}\langle\boldsymbol{\xi},\boldsymbol{x}\rangle}\,\mathrm{d}\boldsymbol{x},\ \ \mathscr{F}^{-1}[\hat{u}](\boldsymbol{x}) = \frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d}\hat{u}(\boldsymbol{\xi})\,\mathrm{e}^{\mathrm{i}\langle\boldsymbol{\xi},\boldsymbol{x}\rangle}\,\mathrm{d}\boldsymbol{\xi}. \tag{2.27}$$

Moreover, the use of A-GHFs as basis functions in a spectral-Galerkin framework can diagonalise the nonlocal integral fractional Laplacian $(-\Delta)^s$ for $s > 0$. Recall that for $s > 0$, the fractional Laplacian of $u \in \mathscr{S}(\mathbb{R}^d)$ (functions of Schwartz class) can be naturally defined via the Fourier transform:

$$(-\Delta)^s u(\boldsymbol{x}) = \mathscr{F}^{-1}\big[|\boldsymbol{\xi}|^{2s}\mathscr{F}[u](\boldsymbol{\xi})\big](\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^d. \tag{2.28}$$

For $0 < s < 1$, the fractional Laplacian can be equivalently defined by the point-wise formula (*cf.* [13]):

$$(-\Delta)^s u(\boldsymbol{x}) = C_{d,s}\,\text{p.v.} \int_{\mathbb{R}^d} \frac{u(\boldsymbol{x}) - u(\boldsymbol{y})}{|\boldsymbol{x} - \boldsymbol{y}|^{d+2s}}\,\mathrm{d}\boldsymbol{y}, \quad C_{d,s} := \frac{2^{2s} s\Gamma(s + d/2)}{\pi^{d/2}\Gamma(1 - s)}, \tag{2.29}$$

where "*p.v.*" stands for the principle value.

Theorem 2.10. *For $\mu > -\frac{1}{2}, (\ell, n) \in \Upsilon_\infty^d$ and $k \in \mathbb{N}_0$, we have*

$$\mathscr{F}[\check{H}^{\mu,n}_{k,\ell}](\boldsymbol{\xi}) = (-\mathrm{i})^{n+2k}\,\widehat{H}^{\mu,n}_{k,\ell}(\boldsymbol{\xi}), \quad \mathscr{F}^{-1}[\widehat{H}^{\mu,n}_{k,\ell}](\boldsymbol{x}) = \mathrm{i}^{n+2k}\,\check{H}^{\mu,n}_{k,\ell}(\boldsymbol{x}), \tag{2.30}$$

and for $s > 0$,

$$\mathscr{F}[(-\Delta)^s\check{H}^{\mu,n}_{k,\ell}](\boldsymbol{\xi}) = (-\mathrm{i})^{n+2k}|\boldsymbol{\xi}|^{2s}\,\widehat{H}^{\mu,n}_{k,\ell}(\boldsymbol{\xi}). \tag{2.31}$$

Moreover, the adjoint GHFs are orthonormal in the sense that for $s > 0$,

$$\big((-\Delta)^{\frac{s}{2}}\check{H}^{s,n}_{k,\ell}, (-\Delta)^{\frac{s}{2}}\check{H}^{s,m}_{j,\iota}\big)_{\mathbb{R}^d} = \delta_{jk}\delta_{mn}\delta_{\ell\iota}. \tag{2.32}$$

Proof. We first show that the GHFs with $\mu = 0$ are eigenfunctions of the Fourier transform, namely,

$$\mathscr{F}[\widehat{H}^{0,n}_{k,\ell}](\boldsymbol{\xi}) = (-\mathrm{i})^{n+2k}\,\widehat{H}^{0,n}_{k,\ell}(\boldsymbol{\xi}). \tag{2.33}$$

According to Lemma 9.10.2 of [2], we have that for $\omega > 0$,

$$\int_{\mathbb{S}^{d-1}} Y^n_\ell(\hat{\boldsymbol{x}})\,\mathrm{e}^{-\mathrm{i}\omega\langle\hat{\boldsymbol{\xi}},\hat{\boldsymbol{x}}\rangle}\mathrm{d}\sigma(\hat{\boldsymbol{x}}) = \frac{(-\mathrm{i})^n(2\pi)^{\frac{d}{2}}}{\omega^{\frac{d-2}{2}}} J_{n+\frac{d-2}{2}}(\omega)\,Y^n_\ell(\hat{\boldsymbol{\xi}}), \quad \hat{\boldsymbol{\xi}} \in \mathbb{S}^{d-1}, \tag{2.34}$$

where $J_\nu(z)$ is the Bessel functions of the first kind of order ν. Then using Definition 2.1 with $\mu = 0$, and (2.34) with $\omega = \rho r$ and $\rho = |\boldsymbol{\xi}|$, leads to

$$\begin{aligned}
\mathscr{F}[\widehat{H}^{0,n}_{k,\ell}](\boldsymbol{\xi}) &= \frac{1}{(2\pi)^{\frac{d}{2}}}\int_{\mathbb{R}^d}\widehat{H}^{0,n}_{k,\ell}(\boldsymbol{x})\mathrm{e}^{-\mathrm{i}\langle\boldsymbol{\xi},\boldsymbol{x}\rangle}\mathrm{d}\boldsymbol{x}\\
&= \frac{1}{\sqrt{\gamma^{0,d}_{k,n}}}\frac{1}{(2\pi)^{\frac{d}{2}}}\int_0^\infty r^n L_k^{(n+\frac{d-2}{2})}(r^2)\mathrm{e}^{-\frac{r^2}{2}}\bigg\{\int_{\mathbb{S}^{d-1}} Y^n_\ell(\hat{\boldsymbol{x}})\mathrm{e}^{-\mathrm{i}\rho r\langle\hat{\boldsymbol{\xi}},\hat{\boldsymbol{x}}\rangle}\mathrm{d}\sigma(\hat{\boldsymbol{x}})\bigg\} r^{d-1}\,\mathrm{d}r\\
&= \frac{1}{\sqrt{\gamma^{0,d}_{k,n}}}\frac{(-\mathrm{i})^n}{\rho^{\frac{d-2}{2}}}\bigg\{\int_0^\infty r^{n+\frac{d}{2}} L_k^{(n+\frac{d-2}{2})}(r^2)\,\mathrm{e}^{-\frac{r^2}{2}}\,J_{n+\frac{d-2}{2}}(\rho r)\,\mathrm{d}r\bigg\} Y^n_\ell(\hat{\boldsymbol{\xi}}), \quad \rho > 0.
\end{aligned} \tag{2.35}$$

Recall the integral identity of the generalised Laguerre polynomials (*cf.* [17], p. 820): for $\alpha > -1$,

$$\int_0^\infty r^{\alpha+1} L_k^{(\alpha)}(r^2)\,\mathrm{e}^{-\frac{r^2}{2}}\,J_\alpha(\rho r)\,\mathrm{d}r = (-1)^k\rho^\alpha L_k^{(\alpha)}(\rho^2)\,\mathrm{e}^{-\frac{\rho^2}{2}}, \quad \rho > 0. \tag{2.36}$$

Thus, taking $\alpha = n + \frac{d-2}{2}$ in (2.36), we can work out the integral in (2.35) and then obtain from (2.13) with $\mu = 0$ that

$$\mathscr{F}[\widehat{H}^{0,n}_{k,\ell}](\boldsymbol{\xi}) = \frac{(-1)^k}{\sqrt{\gamma^{0,d}_{k,n}}}\frac{(-\mathrm{i})^n}{\rho^{\frac{d-2}{2}}}\rho^{n+\frac{d-2}{2}} L_k^{(n+\frac{d-2}{2})}(\rho^2)\mathrm{e}^{-\frac{\rho^2}{2}}\,Y^n_\ell(\hat{\boldsymbol{\xi}}) = (-\mathrm{i})^{n+2k}\,\widehat{H}^{0,n}_{k,\ell}(\boldsymbol{\xi}). \tag{2.37}$$

This yields (2.33).

From Definition 2.8 and the property (2.37), we obtain

$$\begin{aligned}\mathscr{F}[\check{H}^{\mu,n}_{k,\ell}](\boldsymbol{\xi}) &= \sum_{j=0}^{k}(-1)^{k-j}\,{}^{\mu}_{0}\mathbb{C}^{k}_{j}\,\mathscr{F}[\widehat{H}^{0,n}_{j,\ell}](\boldsymbol{\xi}) = \sum_{j=0}^{k}(-1)^{k-j}\,(-\mathrm{i})^{n+2j}\,{}^{\mu}_{0}\mathbb{C}^{k}_{j}\,\widehat{H}^{0,n}_{j,\ell}(\boldsymbol{\xi})\\ &= (-\mathrm{i})^{n+2k}\sum_{j=0}^{k}{}^{\mu}_{0}\mathbb{C}^{k}_{j}\,\widehat{H}^{0,n}_{j,\ell}(\boldsymbol{\xi}) = (-\mathrm{i})^{n+2k}\widehat{H}^{\mu,n}_{k,\ell}(\boldsymbol{\xi}),\end{aligned}\tag{2.38}$$

where in the last step, we used (2.26). This gives the first identity in (2.30), and the second is its immediate consequence. The property (2.31) follows directly from (2.30) and the definition of fractional Laplacian (2.28).

Finally, using the Parseval's identity and (2.31), we derive from the orthogonality (2.15) that

$$\begin{aligned}\big((-\Delta)^{\frac{s}{2}}\check{H}^{s,n}_{k,\ell},(-\Delta)^{\frac{s}{2}}\check{H}^{s,m}_{j,\iota}\big)_{\mathbb{R}^d} &= \big(\mathscr{F}[(-\Delta)^{\frac{s}{2}}\check{H}^{s,n}_{k,\ell}],\mathscr{F}[(-\Delta)^{\frac{s}{2}}\check{H}^{s,m}_{j,\iota}]\big)_{\mathbb{R}^d}\\ &= (-\mathrm{i})^{n-m+2k-2j}(|\boldsymbol{\xi}|^{2s}\widehat{H}^{s,n}_{k,\ell},\widehat{H}^{s,m}_{j,\iota})_{\mathbb{R}^d} = \delta_{mn}\delta_{kj}\delta_{\ell\iota}.\end{aligned}$$

This yields (2.32) and ends the proof. □

Note that the GHFs are real-valued, so we infer from (2.27) readily that

$$\mathscr{F}[\widehat{H}^{\mu,n}_{k,\ell}(\boldsymbol{x})](\boldsymbol{\xi}) = \big\{\mathscr{F}^{-1}[\widehat{H}^{\mu,n}_{k,\ell}(\boldsymbol{x})](\boldsymbol{\xi})\big\}^{*}.$$

Thus, we find from (2.30) immediately the following "reversed" form of (2.30).

Corollary 2.11. *For $\mu > -\frac{1}{2}, (\ell,n)\in\Upsilon^d_\infty$ and $k\in\mathbb{N}_0$, we have*

$$\mathscr{F}[\widehat{H}^{\mu,n}_{k,\ell}](\boldsymbol{\xi}) = \mathrm{i}^{n+2k}\check{H}^{\mu,n}_{k,\ell}(\boldsymbol{\xi}),\quad \mathscr{F}^{-1}[\check{H}^{\mu,n}_{k,\ell}](\boldsymbol{x}) = (-\mathrm{i})^{n+2k}\widehat{H}^{\mu,n}_{k,\ell}(\boldsymbol{x}).\tag{2.39}$$

Remark 2.12. The fractional Sobolev orthogonality (2.32) has profound implications even for the integral-order Laplacian $(-\Delta)^m$ with $m\in\mathbb{N}$. For example, we find from (2.25) with $s=1$ that the A-GHFs read

$$\check{H}^{1,n}_{k,\ell}(\boldsymbol{x}) = \sqrt{\frac{k!}{\Gamma(k+n+\frac{d}{2}+1)}}\sum_{j=0}^{k}\sqrt{\frac{\Gamma(j+n+\frac{d}{2})}{j!}}\,\widehat{H}^{0,n}_{j,\ell}(\boldsymbol{x}),$$

which are orthogonal with respect to $(\nabla\cdot,\nabla\cdot)_{\mathbb{R}^d}$. However, this attractive property is not valid for the usual Hermite-based methods based on tensorial Hermite functions $\prod_{j=1}^{d}\widehat{H}_{n_j}(x_j)$. Thus, it is advantageous to use the A-GHFs for usual Laplacian and bi-harmonic Laplacian (using the A-GHFs with $s=2$) in $\mathbb{R}^d$. □

2.4. Differences and connections with some existing generalisations

There have been some existing generalisations of the usual Hermite polynomials/functions in different senses, so we feel compelled to point out the differences and connections between the GHPs/GHFs herein and some most relevant ones in literature.

2.4.1. GHPs/GHFs in Szegö [43]

Note from (2.6) that for $d=1$, $a^1_0 = a^1_1 = 1$ and $a^1_n = 0$ for $n\geqslant 2$, so there are only two orthonormal harmonic polynomials: $Y^0_1(x) = \frac{1}{\sqrt{2}}$ and $Y^1_1(x) = \frac{x}{\sqrt{2}}$. Accordingly, the GHPs in Definition 2.1 (with a constant multiple) reduce to

$$\begin{aligned}H^{(\mu)}_{2k}(x) &:= (-1)^k\,2^{2k+\frac{1}{2}}\,k!\,H^{\mu,0}_{k,1}(x) = (-1)^k\,2^{2k}\,k!\,L^{(\mu-\frac{1}{2})}_{k}(x^2),\\ H^{(\mu)}_{2k+1}(x) &:= (-1)^k\,2^{2k+\frac{3}{2}}\,k!\,H^{\mu,1}_{k,1}(x) = (-1)^k\,2^{2k+1}\,k!\,x\,L^{(\mu+\frac{1}{2})}_{k}(x^2),\end{aligned}\tag{2.40}$$

which are mutually orthogonal with respect to the weight function $|x|^{2\mu}\,\mathrm{e}^{-x^2}$ on $\mathbb{R}$. In fact, this family of GHPs is first introduced by Szegö in ([43], p. 371) as an exercised problem and promoted by Chihara [10,11]. According to Szegö Problem 25 of [43], the GHPs with $\mu > -\frac{1}{2}$ satisfy the differential equation:

$$xy'' + 2(\mu - x^2)y' + (2nx - \theta_n x^{-1})y = 0, \quad \theta_n = \begin{cases} 0, & n \text{ even}\,, \\ 2\mu, & n \text{ odd}\,; \end{cases} \; y = H_n^{(\mu)}(x). \tag{2.41}$$

Some other properties of $\{H_n^{(\mu)}\}$ can be founded in [10,11]. We also refer to some limited works on the analytic studies or further generalisations (see, *e.g.,* [30,36]). With the normalisation in (2.40), the orthonormal GHFs (in (2.13) with $d = 1$) take the form

$$\widehat{H}_n^{(\mu)}(x) := \sqrt{1/\gamma_n^{(\mu)}}\;\mathrm{e}^{-\frac{x^2}{2}}\,H_n^{(\mu)}(x), \quad \gamma_n^{(\mu)} := 2^{2n}\left[\frac{n}{2}\right]!\,\Gamma\Big(\Big[\frac{n+1}{2}\Big] + \mu + \frac{1}{2}\Big). \tag{2.42}$$

In particular, for $\mu = 0$, they reduce to the usual Hermite polynomials/functions. For distinction, we denote them by $H_n(x)$ and $\widehat{H}_n(x)$, respectively.

From (2.20) and (2.40), we have the following transformation between GHFs with different parameters

$$\widehat{H}_n^{(\mu)}(x) = \sum_{\substack{j=0 \\ j+n \text{ even}}}^{n} {}^{\mu}_{\nu}\widehat{C}^{n}_{j}\;\widehat{H}_j^{(\nu)}(x), \tag{2.43}$$

where for even $j + n$, the connection coefficients are given by

$${}^{\mu}_{\nu}\widehat{C}^{n}_{j} = \frac{(-1)^{\frac{n-j}{2}}\sqrt{\Gamma([\frac{n}{2}]+1)\Gamma([\frac{j+1}{2}]+\nu+\frac{1}{2})}\;\Gamma\big(\frac{n-j}{2}+\mu-\nu\big)}{\Gamma(\mu-\nu)\sqrt{\Gamma([\frac{n+1}{2}]+\mu+\frac{1}{2})\Gamma([\frac{j}{2}]+1)}\;\Gamma\big(\frac{n-j}{2}+1\big)}. \tag{2.44}$$

It is known that the usual Hermite functions $\{\widehat{H}_n\}$ are the eigenfunctions of the Fourier transform. However, this property cannot carry over to the GHFs with $\mu \neq 0$. In ([30] (2.34)), the Fourier transform of $\widehat{H}_n^{(\mu)}(x)$ is expressed in terms of the Kummer hypergeometric function ${}_1F_1(\cdot)$. Here we find from Corollary 2.11 with $d = 1$ the following more informative representation

$$\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \widehat{H}_n^{(\mu)}(x)\mathrm{e}^{-\mathrm{i}\xi x}\mathrm{d}x = \mathrm{i}^n\,\breve{H}_n^{(\mu)}(\xi), \quad \xi \in \mathbb{R}, \tag{2.45}$$

where the one-dimensional adjoint GHFs are given by

$$\breve{H}_n^{(\mu)}(x) = \sum_{\substack{j=0 \\ j+n \text{ even}}}^{n} (-1)^{\frac{n-j}{2}}\;{}^{\mu}_{0}\widehat{C}^{n}_{j}\;\widehat{H}_j(x), \quad x \in \mathbb{R}. \tag{2.46}$$

We remark that the formulation (2.46) requires some simple calculation from (2.25) and (2.40).

2.4.2. 2D GHFs versus generalised Hermite bases for Bose-Einstein condensates in [4]

For $d = 2$, the dimensionality of the space $\mathcal{H}_n^2$ in (2.6) is $a_n^2 = 2 - \delta_{n0}$, with the orthogonal basis given by the real and imaginary parts of $(x_1 + \mathrm{i}x_2)^n$. In polar coordinates, we have

$$Y_1^0(\boldsymbol{x}) = \frac{1}{\sqrt{2\pi}}, \quad Y_1^n(\boldsymbol{x}) = \frac{r^n}{\sqrt{\pi}}\cos(n\theta), \quad Y_2^n(\boldsymbol{x}) = \frac{r^n}{\sqrt{\pi}}\sin(n\theta), \quad n \geqslant 1. \tag{2.47}$$

Then by (2.13), the GHFs can be expressed as

$$\widehat{H}_{k,1}^{\mu,0}(\boldsymbol{x}) = \frac{1}{\sqrt{2\pi\gamma_{k,0}^{\mu,2}}}\, \mathrm{e}^{-\frac{r^2}{2}} L_k^{(\mu)}(r^2), \quad \widehat{H}_{k,1}^{\mu,n}(\boldsymbol{x}) = \frac{1}{\sqrt{\pi\gamma_{k,n}^{\mu,2}}}\, r^n\, \mathrm{e}^{-\frac{r^2}{2}} L_k^{(n+\mu)}(r^2)\cos(n\theta),$$
$$\widehat{H}_{k,2}^{\mu,n}(\boldsymbol{x}) = \frac{1}{\sqrt{\pi\gamma_{k,n}^{\mu,2}}}\, r^n\, \mathrm{e}^{-\frac{r^2}{2}} L_k^{(n+\mu)}(r^2)\sin(n\theta), \quad n \geqslant 1, \;\; k \geqslant 0. \tag{2.48}$$

Note that similar constructions for the 2D GHFs with $\mu = 0$ have been explored in the computation of the ground states and dynamics of Bose-Einstein condensation (*cf.* [4]), governed by the Gross-Pitaevskii equation with an angular momentum rotation term:

$$\mathrm{i}\partial_t\psi(\boldsymbol{x},t) = \Big(-\frac{1}{2}\Delta + \frac{\gamma^2}{2}|\boldsymbol{x}|^2 + \Omega L_z + \beta|\psi(\boldsymbol{x},t)|^2\Big)\psi(\boldsymbol{x},t), \;\; \boldsymbol{x}\in\mathbb{R}^2, \; t>0,$$
$$\psi(\boldsymbol{x},0) = \psi_0(\boldsymbol{x}), \;\; \boldsymbol{x}\in\mathbb{R}^2; \quad \psi(\boldsymbol{x},t)\to 0 \;\text{ as }\; |\boldsymbol{x}|\to\infty, \quad t\geqslant 0, \tag{2.49}$$

where the constants $\gamma, \beta > 0$, Ω is the dimensionless angular momentum rotation speed and $L_z = -\mathrm{i}(x\partial_y - y\partial_x) = -\mathrm{i}\partial_\theta$ in polar coordinates. The efficient spectral algorithm therein was built upon the constructive basis $\{r^n \mathrm{e}^{-\frac{\gamma r^2}{2}} L_k^{(n)}(\gamma r^2)\mathrm{e}^{\mathrm{i}m\theta}\}$ that could diagonalise the Schrödinger operator: $-\Delta + \gamma|\boldsymbol{x}|^2$. Similar idea was extended to (2.49) in $\mathbb{R}^3$ in cylindrical coordinates by using the tensor product of the 2D basis and the usual Hermite function in the z-direction in [4].

In view of Lemma 2.7, the GHFs with $\mu = 0$ are eigenfunctions of the harmonic oscillator: $-\Delta + |\boldsymbol{x}|^2$, so with a proper scaling, the spectral algorithm leads to a diagonal matrix for the scaled harmonic oscillator: $-\Delta + \gamma^2|\boldsymbol{x}|^2$. As we shall show in the late part, our GHFs with $\mu \neq 0$ offer a new and efficient tool for the solutions of PDEs involving a more general Schrödinger operator: $(-\Delta)^s + |\boldsymbol{x}|^{2\mu}$ with $s \in (0,1]$ and $\mu > -1/2$.

2.4.3. 3D GHPs versus Burnett polynomials [8]

For $d = 3$, the dimensionality of $\mathcal{H}_n^3$ in (2.6) is $a_n^3 = 2n+1$. The orthonormal basis in the spherical coordinates $\boldsymbol{x} = (r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta)^t$ takes the form

$$Y_1^n(\boldsymbol{x}) = \frac{1}{\sqrt{8\pi}} P_n^{(0,0)}(\cos\theta); \;\; Y_{2l}^n(\boldsymbol{x}) = \frac{r^n}{2^{l+1}\sqrt{\pi}}(\sin\theta)^l P_{n-l}^{(l,l)}(\cos\theta)\cos(l\phi),$$
$$Y_{2l+1}^n(\boldsymbol{x}) = \frac{r^n}{2^{l+1}\sqrt{\pi}}(\sin\theta)^l P_{n-l}^{(l,l)}(\cos\theta)\sin(l\phi), \quad 1\leqslant l\leqslant n, \tag{2.50}$$

where $\{P_k^{(l,l)}\}$ are the Gegenbauer polynomials. Then the 3D GHPs/GHFs in Definition 2.1 read more explicit. In fact, for $\mu = 0$, the GHPs with a scaling turn out to be the Burnett polynomials, which were first proposed by Burnett [8] as follows

$$B_{k,\ell}^n(\boldsymbol{x}) = c_k^n \, r^n L_k^{(n+\frac{1}{2})}\Big(\frac{r^2}{2}\Big) Y_\ell^n(\hat{\boldsymbol{x}}), \quad k\in\mathbb{N}_0, \; (\ell,n)\in\Upsilon_\infty^3, \tag{2.51}$$

where c_k^n is the normalisation constant so that they are orthogonal in the sense

$$\int_{\mathbb{R}^3} B_{k,\ell}^n(\boldsymbol{x})\, B_{j,\iota}^m(\boldsymbol{x})\, \mathrm{e}^{-\frac{|\boldsymbol{x}|^2}{2}}\, \mathrm{d}\boldsymbol{x} = \delta_{kj}\delta_{mn}\delta_{\ell\iota}. \tag{2.52}$$

As a result, the Burnett polynomials are mutually orthogonal with respect to the Maxwellian $\mathcal{M}(\boldsymbol{x}) = \frac{1}{(2\pi)^{3/2}}\mathrm{e}^{-\frac{|\boldsymbol{x}|^2}{2}}$. It is evident that by (2.12) and (2.14) (with $d = 3$ and $\mu = 0$),

$$H_{k,\ell}^{0,n}(\boldsymbol{x}) = \tilde{c}_k^n\, B_{k,\ell}^n(\sqrt{2}\boldsymbol{x}), \quad \boldsymbol{x}\in\mathbb{R}^3. \tag{2.53}$$

We remark that the Burnett polynomials are frequently used as basis functions in solving kinetic equations (*cf.* [9, 20] and the references therein).

2.4.4. Differences with Hagedorn wavepackets [18] and some other generalisations [46]

The Hagedorn wavepackets first introduced in [18] are deemed as an effective numerical tool in computing quantum dynamics (see [24] for an up-to-date review). They generalise the usual Hermite functions to several dimensions that allow for flexible localisation in position and momentum. According to [23], the Hagedorn wavepackets are constructed from the complex Gaussian function:

$$\varphi_0^\varepsilon(\boldsymbol{x}) = (\pi\varepsilon)^{\frac{d}{4}} \det(\boldsymbol{Q})^{-1/2} \exp\Big(\frac{\mathrm{i}}{2\varepsilon}(\boldsymbol{x}-\boldsymbol{q})^T \boldsymbol{P}\boldsymbol{Q}^{-1}(\boldsymbol{x}-\boldsymbol{q}) + \frac{\mathrm{i}}{\varepsilon}\boldsymbol{p}^T(\boldsymbol{x}-\boldsymbol{q})\Big),$$

centred in position $\boldsymbol{p} \in \mathbb{R}^d$ and momentum $\boldsymbol{q} \in \mathbb{R}^d$, where $\boldsymbol{P}, \boldsymbol{Q} \in \mathbb{C}^{d\times d}$ are complex matrices satisfying certain symplecticity conditions, and $0 < \varepsilon \ll 1$ is the semiclassical scaling parameter in the time-dependent Schrödinger equation. Then applying the Hagedorns raising operator $\boldsymbol{k} = (k_1, \cdots, k_d)$-fold to $\varphi_0^\varepsilon(\boldsymbol{x})$ leads to the Hagedorn wavepackets, which can be represented as a product of the multivariate tensorial Hermite polynomials $p_{\boldsymbol{k}}(\boldsymbol{x})$ (with an appropriate scaling) and the initial complex Gaussian function as follows

$$\varphi_{\boldsymbol{k}}^\varepsilon(\boldsymbol{x}) = \frac{1}{\sqrt{2|\boldsymbol{k}|\boldsymbol{k}!}} p_{\boldsymbol{k}}^\varepsilon(\boldsymbol{x})\varphi_0^\varepsilon(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^d,$$

where $|\boldsymbol{k}| = k_1 + \cdots + k_d$ and $\boldsymbol{k}! = k_1! \cdots k_d!$. We refer to [23, 24] for more details.

Inspired by the work of Hagedorn, the very recent PhD dissertation [46] discussed the extension of the tensorial (usual) Hermite polynomials to the generalised anisotropic Hermite functions of the form

$$H_{\boldsymbol{k}}^{\boldsymbol{G},\boldsymbol{E},t}(\boldsymbol{x}) = \frac{t^{|\boldsymbol{k}|/2}}{\sqrt{2|\boldsymbol{k}|\boldsymbol{k}!}} H_{\boldsymbol{k}}\left(\boldsymbol{G}^T\boldsymbol{x}\right) \exp\left(-\boldsymbol{x}^T\boldsymbol{E}^T\boldsymbol{E}\boldsymbol{x}\right), \tag{2.54}$$

where $\boldsymbol{E}, \boldsymbol{G} \in \mathbb{R}^{d\times d}$ are arbitrary invertible matrices, $t > 0$ is a parameter and $H_{\boldsymbol{k}}(\boldsymbol{x}) = H_{k_1}(x_1)\cdots H_{k_d}(x_d)$ is a tensor product of the univariate (usual) Hermite polynomials. We refer to [46] for interesting applications in the context of quantum dynamics.

It is evident that our nontensorial GHPs/GHFs are very different from the Hagedorn wavepackets and their variances. We also remark that the tensorial GHFs were briefly discussed in ([14], p. 278) under a general framework with the weight function $h_{\boldsymbol{k}}^2(\boldsymbol{x})\mathrm{e}^{-\|\boldsymbol{x}\|^2}$ (where $h_{\boldsymbol{k}}$ is a reflection-invariant weight function).

3. GHF approximation of the IFL and the Schrödinger equation

In this section, we implement and analyse the GHF-spectral-Galerkin method for PDEs involving integral fractional Laplacian.

3.1. GHF-spectral-Galerkin method for a fractional model problem

As an illustrative example, we consider

$$(-\Delta)^s u(\boldsymbol{x}) + \gamma u(\boldsymbol{x}) = f(\boldsymbol{x}) \ \text{ in } \mathbb{R}^d; \quad u(\boldsymbol{x}) \to 0 \ \text{ as } |\boldsymbol{x}| \to \infty, \tag{3.1}$$

where $s \in (0,1), \gamma > 0$, $f \in H^{-s}(\mathbb{R}^d)$, and the fractional Laplacian operator is defined in (2.28)-(2.29). Here, the fractional Sobolev space $H^s(\mathbb{R}^d)$ with real s is defined as in [13].

A weak formulation of (3.1) is to find $u \in H^s(\mathbb{R}^d)$ such that

$$\mathcal{A}_s(u,v) = \big((-\Delta)^{\frac{s}{2}}u, (-\Delta)^{\frac{s}{2}}v\big)_{\mathbb{R}^d} + \gamma(u,v)_{\mathbb{R}^d} = (f,v)_{\mathbb{R}^d}, \quad \forall v \in H^s(\mathbb{R}^d). \tag{3.2}$$

From (2.28), we find readily the continuity and coercivity of the bilinear form $\mathcal{A}_s(\cdot,\cdot)$.

Then we conclude from the standard Lax-Milgram lemma that the problem (3.2) admits a unique solution satisfying $\|u\|_{H^s(\mathbb{R}^d)} \leqslant c\|f\|_{H^{-s}(\mathbb{R}^d)}$.

We choose the finite dimensional approximation space spanned by the d-dimensional GHFs in Definition 2.1 or equivalently by the A-GHFs in Definition 2.8. However, in view of (2.32), it is advantageous to use the latter as the basis functions, so we define

$$\mathcal{V}_N^d := \operatorname{span}\big\{\breve{H}_{k,\ell}^{s,n}(\boldsymbol{x}) : \ 0 \leqslant n \leqslant N, \ 1 \leqslant \ell \leqslant a_n^d, \ 0 \leqslant 2k \leqslant N-n, \ k,\ell,n \in \mathbb{N}_0\big\}. \tag{3.3}$$

Then, the spectral-Galerkin approximation to (3.2) is to find $u_N \in \mathcal{V}_N^d$ such that

$$\mathcal{A}_s(u_N, v_N) = (f, v_N)_{\mathbb{R}^d}, \quad \forall v_N \in \mathcal{V}_N^d. \tag{3.4}$$

As with the continuous problem (3.2), it has a unique solution $u_N \in \mathcal{V}_N^d$.

In the real implementation, we write

$$u_N(\boldsymbol{x}) = \sum_{n=0}^{N} \sum_{\ell=1}^{a_n^d} \sum_{k=0}^{[\frac{N-n}{2}]} \tilde{u}_{k,\ell}^n \breve{H}_{k,\ell}^{s,n}(\boldsymbol{x}), \tag{3.5}$$

and arrange the unknown coefficients in the order

$$\begin{aligned} \boldsymbol{u} &= \big(\tilde{\boldsymbol{u}}_1^0, \tilde{\boldsymbol{u}}_2^0, \cdots, \tilde{\boldsymbol{u}}_{a_0^d}^0, \tilde{\boldsymbol{u}}_1^1, \tilde{\boldsymbol{u}}_2^1, \cdots, \tilde{\boldsymbol{u}}_{a_1^d}^1, \cdots, \tilde{\boldsymbol{u}}_1^N, \tilde{\boldsymbol{u}}_2^N, \cdots, \tilde{\boldsymbol{u}}_{a_N^d}^N\big)^t, \\ \tilde{\boldsymbol{u}}_\ell^n &= \big(\tilde{u}_{0,\ell}^n, \tilde{u}_{1,\ell}^n, \cdots, \tilde{u}_{[\frac{N-n}{2}],\ell}^n\big)^t, \end{aligned} \tag{3.6}$$

and likewise for $\boldsymbol{f}$, but with the components $\tilde{f}_{k,\ell}^n = (f, \breve{H}_{k,\ell}^{s,n})_{\mathbb{R}^d}$. The orthogonality (2.32) implies that the stiffness matrix is an identity matrix. Moreover, in view of the orthogonality of the spherical harmonic basis (*cf.* (2.8)), the corresponding mass matrix is block diagonal as follows

$$\boldsymbol{M} = \operatorname{diag}\big\{\boldsymbol{M}_1^0, \boldsymbol{M}_2^0, \cdots, \boldsymbol{M}_{a_0^d}^0, \boldsymbol{M}_1^1, \boldsymbol{M}_2^1, \cdots, \boldsymbol{M}_{a_1^d}^1, \cdots, \boldsymbol{M}_1^N, \boldsymbol{M}_2^N, \cdots, \boldsymbol{M}_{a_N^d}^N\big\}, \tag{3.7}$$

where the entries of each diagonal block can be computed by

$$\begin{aligned} (\boldsymbol{M}_\ell^n)_{kj} &= \big(\breve{H}_{k,\ell}^{s,n}, \breve{H}_{j,\ell}^{s,n}\big)_{\mathbb{R}^d} = \sum_{p=0}^{k} (-1)^{k-p} \, {}_0^s\mathbb{C}_p^k \sum_{q=0}^{j} (-1)^{j-q} \, {}_0^s\mathbb{C}_q^j \, \big(\widehat{H}_{p,\ell}^{0,n}, \widehat{H}_{q,\ell}^{0,n}\big)_{\mathbb{R}^d} \\ &= (-1)^{k+j} \sum_{p=0}^{\min\{j,k\}} {}_0^s\mathbb{C}_p^k \, {}_0^s\mathbb{C}_p^j \,. \end{aligned} \tag{3.8}$$

Thus the linear system of (3.4) can be written as

$$(\boldsymbol{I} + \gamma \boldsymbol{M})\boldsymbol{u} = \boldsymbol{f}. \tag{3.9}$$

Remark 3.1. With the new basis at our disposal, the above method has remarkable advantages over the existing Hermite approaches (*cf.* [29, 45]). Although the usual one-dimensional Hermite functions are eigenfunctions of the Fourier transform, we observe from (2.28) that the factor $|\boldsymbol{\xi}|^{2s}$ is non-separable and singular, so the use of tensorial Hermite functions leads to a dense stiffness matrix whose entries are difficult to evaluate due to the involved singularity for $d \geqslant 2$. □

3.1.1. Error analysis

Applying the first Strang lemma [42] for the standard Galerkin framework (*i.e.,* (3.2) and (3.4)), we obtain immediately that

$$\|u - u_N\|_{H^s(\mathbb{R}^d)} \leqslant c \inf_{v_N \in \mathcal{V}_N^d} \|u - v_N\|_{H^s(\mathbb{R}^d)} \,. \tag{3.10}$$

To obtain optimal error estimates, we have to resort to some intermediate approximation results related to certain orthogonal projection. To this end, we consider the L^2-orthogonal projection $\pi_N^d : L^2(\mathbb{R}^d) \to \mathcal{V}_N^d$ such that

$$(\pi_N^d u - u, v)_{\mathbb{R}^d} = 0, \quad \forall v \in \mathcal{V}_N^d. \tag{3.11}$$

From Definition 2.8 and with a change of basis functions, we find readily that

$$\mathcal{V}_N^d := \mathrm{span}\big\{\widehat{H}_{k,\ell}^{0,n}(\boldsymbol{x}) : \ 0 \leqslant n \leqslant N, \ 1 \leqslant \ell \leqslant a_n^d, \ 0 \leqslant 2k \leqslant N-n, \ k,\ell,n \in \mathbb{N}_0\big\}. \tag{3.12}$$

Thus, we can equivalently write

$$\pi_N^d u(\boldsymbol{x}) = \sum_{n=0}^{N} \sum_{\ell=1}^{a_n^d} \sum_{k=0}^{[\frac{N-n}{2}]} \hat{u}_{k,\ell}^n \widehat{H}_{k,\ell}^{0,n}(\boldsymbol{x}). \tag{3.13}$$

Based on (2.23), we introduce the function space $\mathcal{B}^r(\mathbb{R}^d)$ equipped with the norm

$$\|u\|_{\mathcal{B}^r(\mathbb{R}^d)}^2 = \begin{cases} \|(-\Delta + |\boldsymbol{x}|^2)^m u\|_{L^2(\mathbb{R}^d)}^2, & r = 2m, \\ \dfrac{1}{2}\big(\|(\boldsymbol{x}+\nabla)(-\Delta + |\boldsymbol{x}|^2)^m u\|_{L^2(\mathbb{R}^d)}^2 + \|(\boldsymbol{x}-\nabla)(-\Delta + |\boldsymbol{x}|^2)^m u\|_{L^2(\mathbb{R}^d)}^2\big), & r = 2m+1, \end{cases} \tag{3.14}$$

where integer $r \geqslant 0$, and $\boldsymbol{x} + \nabla$ and $\boldsymbol{x} - \nabla$ are the lowering and raising operators, respectively.

The main approximation result is stated below.

Theorem 3.2. *Let $s \in (0,1)$. For any $u \in \mathcal{B}^r(\mathbb{R}^d)$ with integer $r \geqslant 1$, we have*

$$\|\pi_N^d u - u\|_{H^s(\mathbb{R}^d)} \leqslant (2N + d + 2)^{(s-r)/2} \|u\|_{\mathcal{B}^r(\mathbb{R}^d)}. \tag{3.15}$$

Proof. (i). We first estimate the L^2-error. For $r = 2m+1$, a direct calculation gives

$$\begin{aligned} \|u\|_{\mathcal{B}^r(\mathbb{R}^d)}^2 &= \frac{1}{2}\Big(\|(\boldsymbol{x}+\nabla)(-\Delta + |\boldsymbol{x}|^2)^m u\|_{L^2(\mathbb{R}^d)}^2 + \|(\boldsymbol{x}-\nabla)(-\Delta + |\boldsymbol{x}|^2)^m u\|_{L^2(\mathbb{R}^d)}^2\Big) \\ &= \big((-\Delta + |\boldsymbol{x}|^2)^{m+1} u, (-\Delta + |\boldsymbol{x}|^2)^m u\big)_{\mathbb{R}^d}. \end{aligned} \tag{3.16}$$

Thanks to the orthogonality (2.15), (2.23)–(3.14) and (3.16), we have that for any $r \geqslant 0$,

$$\|u\|_{\mathcal{B}^r(\mathbb{R}^d)}^2 = \sum_{n=0}^{\infty} \sum_{\ell=1}^{a_n^d} \sum_{k=0}^{\infty} h_{k,d}^{n,r} |\hat{u}_{k,\ell}^n|^2, \quad h_{k,d}^{n,r} = (4k + 2n + d)^r. \tag{3.17}$$

Then, we derive from (3.13) and (3.17) that

$$\begin{aligned} \|\pi_N^d u - u\|_{L^2(\mathbb{R}^d)}^2 &= \sum_{n=0}^{\infty} \sum_{\ell=1}^{a_n^d} \sum_{k=\lceil \frac{N+1-n}{2} \rceil}^{\infty} h_{k,d}^{n,0} |\hat{u}_{k,\ell}^n|^2 \\ &\leqslant \max_{2k+n \geqslant N+1} \left\{ \frac{h_{k,d}^{n,0}}{h_{k,d}^{n,r}} \right\} \sum_{n=0}^{\infty} \sum_{\ell=1}^{a_n^d} \sum_{k=\lceil \frac{N+1-n}{2} \rceil}^{\infty} h_{k,d}^{n,r} |\hat{u}_{k,\ell}^n|^2 \\ &\leqslant (2N + 2 + d)^{-r} \|u\|_{\mathcal{B}^r(\mathbb{R}^d)}^2. \end{aligned} \tag{3.18}$$

If $r = 2m$, we find from (3.14) that (3.16) simply becomes

$$\|u\|_{\mathcal{B}^r(\mathbb{R}^d)}^2 = \big((-\Delta + |\boldsymbol{x}|^2)^m u, (-\Delta + |\boldsymbol{x}|^2)^m u\big)_{\mathbb{R}^d}, \tag{3.19}$$

so we can follow the same lines as above to derive the L^2-estimate.

(ii). We next estimate the H^1-error. Using the triangle inequality and (3.16), we obtain that

$$\begin{aligned}\|\nabla(\pi_N^d u-u)\|^2_{L^2(\mathbb{R}^d)} &\leqslant \frac{1}{2}\Big(\|(\boldsymbol{x}+\nabla)(\pi_N^d u-u)\|^2_{L^2(\mathbb{R}^d)}+\|(\boldsymbol{x}-\nabla)(\pi_N^d u-u)\|^2_{L^2(\mathbb{R}^d)}\Big)\\ &= \big((-\Delta+|\boldsymbol{x}|^2)(\pi_N^d u-u),(\pi_N^d u-u)\big)_{\mathbb{R}^d}\leqslant \sum_{n=0}^{\infty}\sum_{\ell=1}^{a_n^d}\sum_{k=\lceil\frac{N+1-n}{2}\rceil}^{\infty} h_{k,d}^{n,1}|\hat{u}_{k,\ell}^n|^2\\ &\leqslant \max_{2k+n\geqslant N+1}\left\{\frac{h_{k,d}^{n,1}}{h_{k,d}^{n,r}}\right\}\sum_{n=0}^{\infty}\sum_{\ell=1}^{a_n^d}\sum_{k=\lceil\frac{N+1-n}{2}\rceil}^{\infty} h_{k,d}^{n,r}|\hat{u}_{k,\ell}^n|^2\\ &\leqslant (2N+2+d)^{1-r}\|u\|^2_{\mathcal{B}^r(\mathbb{R}^d)}.\end{aligned}\tag{3.20}$$

Finally, the desired results can be obtained by the L^2- and H^1-bounds derived above and the following space interpolation inequality (*cf.* [1], Ch. 1)

$$\|u\|_{H^s(\mathbb{R}^d)}\leqslant \|u\|^{1-s}_{L^2(\mathbb{R}^d)}\,\|u\|^s_{H^1(\mathbb{R}^d)},\quad s\in(0,1).\tag{3.21}$$

This ends the proof. □

Taking $v_N=\pi_N^d u$ in (3.10) and using Theorem 3.2, we immediately obtain the following error estimate.

Theorem 3.3. *Let u and u_N be the solutions to (3.2) and (3.4), respectively. If $u\in\mathcal{B}^r(\mathbb{R}^d)$ with integer $r\geqslant 1$, then we have*

$$\|u-u_N\|_{H^s(\mathbb{R}^d)}\leqslant c(2N+d+2)^{(s-r)/2}\|u\|_{\mathcal{B}^r(\mathbb{R}^d)},\quad s\in(0,1),\tag{3.22}$$

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

3.1.2. Numerical results

We conclude this section with some numerical results. For the convenience of implementation, we fix the degree of the numerical solution in both radial and angular direction in (3.5), so the numerical solution takes the form

$$u_{N,K}(\boldsymbol{x})=\sum_{n=0}^{N}\sum_{\ell=1}^{a_n^d}\sum_{k=0}^{K}\hat{u}_{k,\ell}^n\,\breve{H}_{k,\ell}^{s,n}(\boldsymbol{x}).\tag{3.23}$$

Here, we focus on $d=2,3$.

Example 3.4. (Problem (3.1) with exact solution). We first consider (3.1) with the following exact solutions:

$$u_e(\boldsymbol{x})=\mathrm{e}^{-|\boldsymbol{x}|^2},\quad u_a(\boldsymbol{x})=(1+|\boldsymbol{x}|^2)^{-r},\quad r>0,\ \ \boldsymbol{x}\in\mathbb{R}^d.\tag{3.24}$$

According to Propositions 4.2 & 4.3 of [40], the source terms $f_e(\boldsymbol{x})$ and $f_a(\boldsymbol{x})$ are respectively given by

$$\begin{aligned}f_e(\boldsymbol{x})&=\gamma\mathrm{e}^{-|\boldsymbol{x}|^2}+\frac{2^{2s}\Gamma(s+d/2)}{\Gamma(d/2)}\,{}_1F_1\Big(s+\frac{d}{2};\frac{d}{2};-|\boldsymbol{x}|^2\Big),\\ f_a(\boldsymbol{x})&=\gamma(1+|\boldsymbol{x}|^2)^{-r}+\frac{2^{2s}\Gamma(s+r)\Gamma(s+d/2)}{\Gamma(r)\Gamma(d/2)}\,{}_2F_1\Big(s+r,s+\frac{d}{2};\frac{d}{2};-|\boldsymbol{x}|^2\Big).\end{aligned}$$

For $d=2,3$, we take $s=0.3,\ 0.5,\ 0.7$ and the degree in angular direction is fixed $N\equiv 10$ (see (3.23)). In Figure 1 (c)-(f), we plot the maximum errors, in semi-log scale and log-log scale, for u_e and u_a with $d=2,3$ against various K, respectively. As expected, we observe the exponential and algebraic convergence for u_e and u_a, respectively.

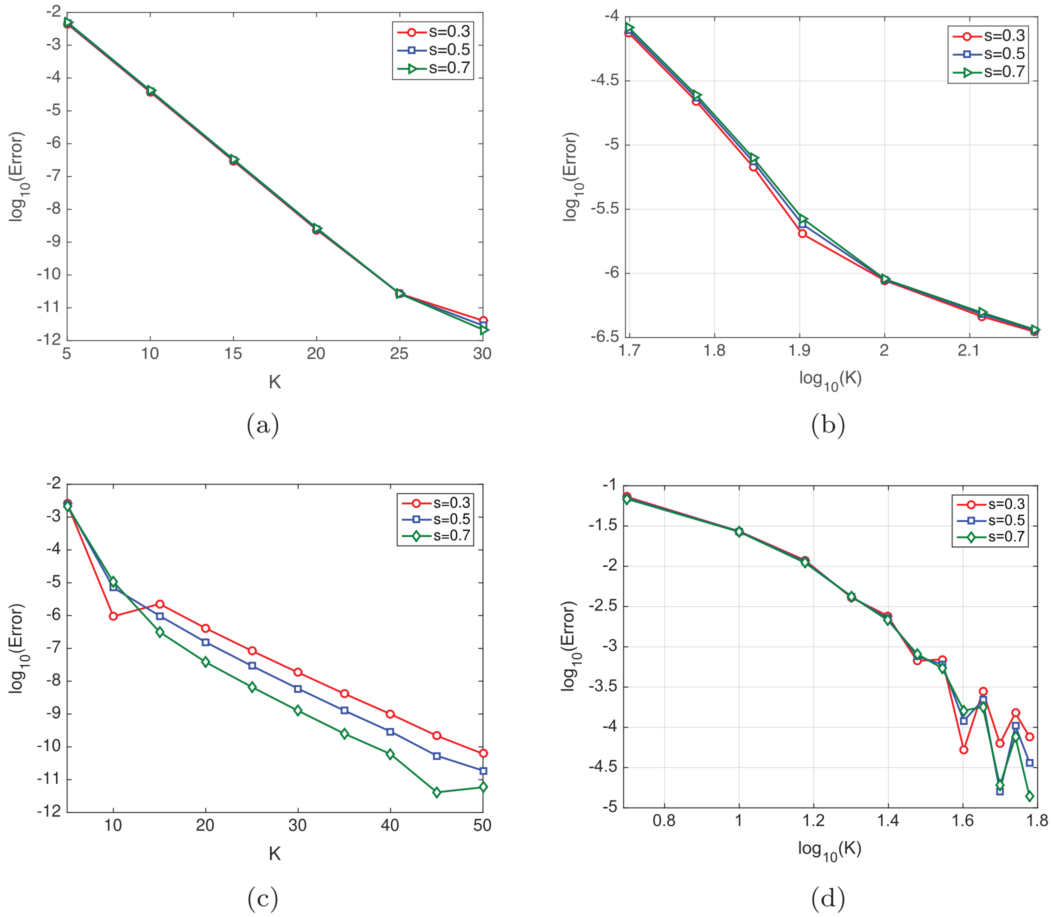


FIGURE 1. The maximum errors of the GHF-spectral-Galerkin scheme with $\gamma = 1$ for Example 3.4 with exact solutions in (3.24). Here $s = 0.3,\ 0.5,\ 0.7$. (a) $d = 2$ and $u_e(\boldsymbol{x}) = e^{-|\boldsymbol{x}|^2}$. (b) $d = 2$ and $u_a(\boldsymbol{x}) = (1+|\boldsymbol{x}|^2)^{-2}$. (c) $d = 3$ and $u_e(\boldsymbol{x}) = e^{-|\boldsymbol{x}|^2}$. (d) $d = 3$ and $u_a(\boldsymbol{x}) = (1+|\boldsymbol{x}|^2)^{-2}$.

Example 3.5. [Problem (3.1) with a source term.] We next consider (3.1) with the following source functions:

$$f_e(\boldsymbol{x}) = \sin(|\boldsymbol{x}|)\mathrm{e}^{-|\boldsymbol{x}|^2}, \quad f_a(\boldsymbol{x}) = \cos(|\boldsymbol{x}|)(1+|\boldsymbol{x}|^2)^{-r}, \quad r > 0, \ \ \boldsymbol{x} \in \mathbb{R}^d. \tag{3.25}$$

The exact solutions are unknown, and we use the numerical solution with $K = 80$, $N = 20$ as the reference solution. For $d = 2, 3$, we plot the maximum errors, in log-log scale, for (3.1) against various K in Figure 2(c)–(f), which we take $s = 0.3,\ 0.5,\ 0.7$ and fix $N \equiv 10$. As shown in [40], the solution of (3.1) decays algebraically, even for exponentially decaying source terms. Indeed, we observe an algebraic order of convergence.

3.2. GHF-spectral-Galerkin method for fractional Schrödinger equations

As a second example, we consider the fractional Schrödinger equation:

$$\begin{aligned} \mathrm{i}\partial_t\psi(\boldsymbol{x},t) &= \Big[\frac{1}{2}(-\Delta)^s + \frac{\gamma^2}{2}|\boldsymbol{x}|^{2\mu}\Big]\psi(\boldsymbol{x},t), \quad \boldsymbol{x} \in \mathbb{R}^2, \ \ t > 0,\\ \psi(\boldsymbol{x},0) &= \psi_0(\boldsymbol{x}), \ \ \boldsymbol{x} \in \mathbb{R}^2; \quad \psi(\boldsymbol{x},t) \to 0 \ \text{ as } \ |\boldsymbol{x}| \to \infty, \quad t \geqslant 0, \end{aligned} \tag{3.26}$$

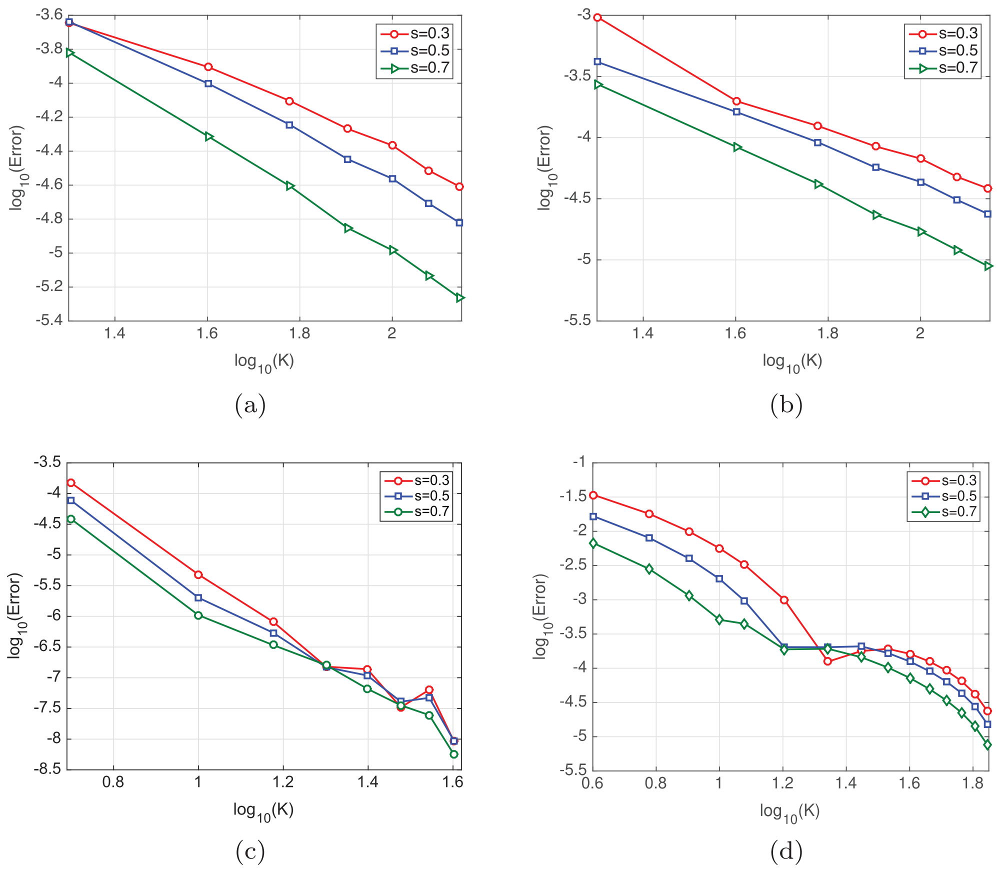


FIGURE 2. The maximum errors of the GHF-spectral-Galerkin scheme with $\gamma = 1$ for Example 3.5 with given source functions in (3.25). Here $s = 0.3,\ 0.5,\ 0.7$ and $r = 2$. (a) $d = 2$ with given source term $f_e(\boldsymbol{x})$. (b) $d = 2$ with given source term $f_a(\boldsymbol{x})$. (c) $d = 3$ with given source term $f_e(\boldsymbol{x})$. (d) $d = 3$ with given source term $f_a(\boldsymbol{x})$.

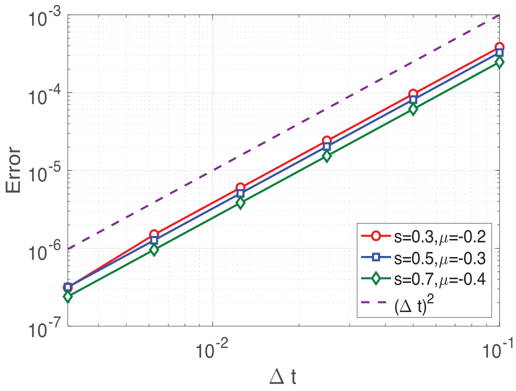
where $s \in (0,1]$, $\mu > -1/2$, the constant $\gamma > 0$, and the function ψ_0 is given. Here, we focus on the linear equation. Indeed, using a suitable time-splitting scheme, one only needs to solve a linear Schrödinger equation at each time step for some typical nonlinear cases (see, *e.g.,* [4]). We remark that the fractional Schrödinger Equation (3.26) is the model of interest in the study of fractional quantum mechanics, see [22,47], where in [22], this fractional Hamiltonian appeared more reasonable to study the problem of quarkonium.

To solve (3.26) efficiently, we adopt the A-GHFs spectral method in space and the Crank-Nicolson scheme in time discretization. Let Δt be the time-stepping size, and $\psi^k(\boldsymbol{x}) \approx \psi(\boldsymbol{x}, k\Delta t)$. Then we look for $\psi^{n+1} \in H^s(\mathbb{R}^2)$ such that

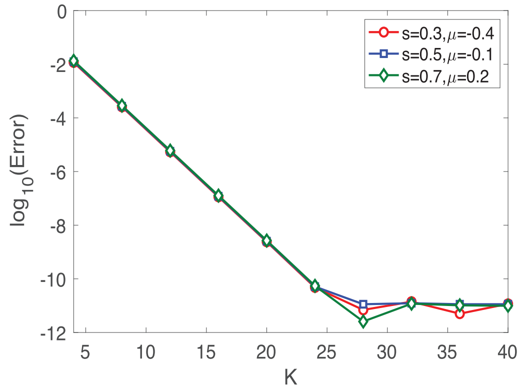
$$\mathrm{i}\Big(\frac{\psi^{n+1} - \psi^n}{\Delta t}, v\Big)_{\mathbb{R}^2} = \frac{1}{2}\big((-\Delta)^{\frac{s}{2}}\psi^{n+\frac{1}{2}}, (-\Delta)^{\frac{s}{2}}v\big)_{\mathbb{R}^2} + \frac{\gamma^2}{2}(|\boldsymbol{x}|^{2\mu}\psi^{n+\frac{1}{2}}, v)_{\mathbb{R}^2}, \quad \forall v \in H^s(\mathbb{R}^2), \tag{3.27}$$

where $\psi^{n+\frac{1}{2}} = (\psi^{n+1} + \psi^n)/2$. We can implement the GHF-spectral scheme as with the problem (3.4), but only need to evaluate the matrix $\boldsymbol{V}$ associated with the potential $|\boldsymbol{x}|^{2\mu}$. It is a block diagonal matrix

$$\boldsymbol{V} = \mathrm{diag}\{\boldsymbol{V}_1^0, \boldsymbol{V}_2^0, \cdots, \boldsymbol{V}_{a_0^d}^0, \boldsymbol{V}_1^1, \boldsymbol{V}_2^1, \cdots, \boldsymbol{V}_{a_1^d}^1, \cdots, \boldsymbol{V}_1^N, \boldsymbol{V}_2^N, \cdots, \boldsymbol{V}_{a_N^d}^N\}, \tag{3.28}$$



(a)



(b)

FIGURE 3. (a) The temporal errors for Crank-Nicolson scheme at $t = 1$ with different s, μ; (b) The spatial errors of GHF-spectral-Galerkin method at $t = 1$ with different s, μ.

and the entries of each diagonal block can be evaluated explicitly by using (2.15), (2.20) and (2.25):

$$\begin{aligned}(\boldsymbol{V}_\ell^n)_{kj} &= \big(|\boldsymbol{x}|^{2\mu} \check{H}^{s,n}_{k,\ell}, \check{H}^{s,n}_{j,\ell}\big)_{\mathbb{R}^d} = \sum_{p=0}^{k} (-1)^{k-p}\, {}^{s}_{0}\mathbb{C}^k_p \sum_{q=0}^{j} (-1)^{j-q}\, {}^{s}_{0}\mathbb{C}^j_q \left(|\boldsymbol{x}|^{2\mu} \widehat{H}^{0,n}_{p,\ell}, \widehat{H}^{0,n}_{q,\ell}\right)_{\mathbb{R}^d} \\ &= \sum_{p=0}^{k} (-1)^{k-p}\, {}^{s}_{0}\mathbb{C}^k_p \sum_{q=0}^{j} (-1)^{j-q}\, {}^{s}_{0}\mathbb{C}^j_q \sum_{p'=0}^{p} {}^{0}_{\mu}\mathbb{C}^p_{p'} \sum_{q'=0}^{q} {}^{0}_{\mu}\mathbb{C}^q_{q'} \left(|\boldsymbol{x}|^{2\mu} \widehat{H}^{\mu,n}_{p',\ell}, \widehat{H}^{\mu,n}_{q',\ell}\right)_{\mathbb{R}^d} \\ &= \sum_{p=0}^{k} (-1)^{k-p}\, {}^{s}_{0}\mathbb{C}^k_p \sum_{q=0}^{j} (-1)^{j-q}\, {}^{s}_{0}\mathbb{C}^j_q \sum_{p'=0}^{p} {}^{0}_{\mu}\mathbb{C}^p_{p'} \sum_{q'=0}^{q} {}^{0}_{\mu}\mathbb{C}^q_{q'}. \end{aligned} \tag{3.29}$$

To test the accuracy of the proposed method, we add an external source term $f(\boldsymbol{x}, t)$ so that the exact solution is $\psi(\boldsymbol{x}, t) = \mathrm{e}^{-|\boldsymbol{x}|^2 - t}$. In Figure 3 (a), we plot the maximum errors *versus* Δt at $t = 1$, and the second-order convergence is observed. Here we take $\gamma = 1$, $N = 10$, $K = 50$ and different s, μ. We choose the time stepping size to be small so that the error is dominated by the spatial error. In Figure 3(b), we plot maximum errors in the semi-log scale *versus* various K, for which we take $N = 10$, $\gamma = 1$ and different s, μ. We observe that the spatial errors decay exponentially as K increases.

Next, we investigate the dynamics of beam propagations as in [47] (where the case $\mu = 1$ was considered). We take the following incident Gaussian beam as the initial condition:

$$\psi(\boldsymbol{x}, 0) = \psi_0(\boldsymbol{x}) = \mathrm{e}^{-\sigma|\boldsymbol{x}|^2 - \mathrm{i}C|\boldsymbol{x}|}, \tag{3.30}$$

where the constants σ and C are the beam width and the linear chirp coefficient, respectively. In the test, we take $\sigma = C = 1$. In Figure 4, we depict the profiles of the real part of the numerical solutions for various s, μ at $t = 2$. Figure 4 (a) shows the solution profile of the usual case with a harmonic potential: $-\Delta + |\boldsymbol{x}|^2$ for comparison. We observe from the other profiles that the solutions have different peak intensities and singular behaviours, from which we find the smaller the value of μ, and the stronger the singularity. In fact, some similar observations was made in [47] for the case with $\mu = 1$.

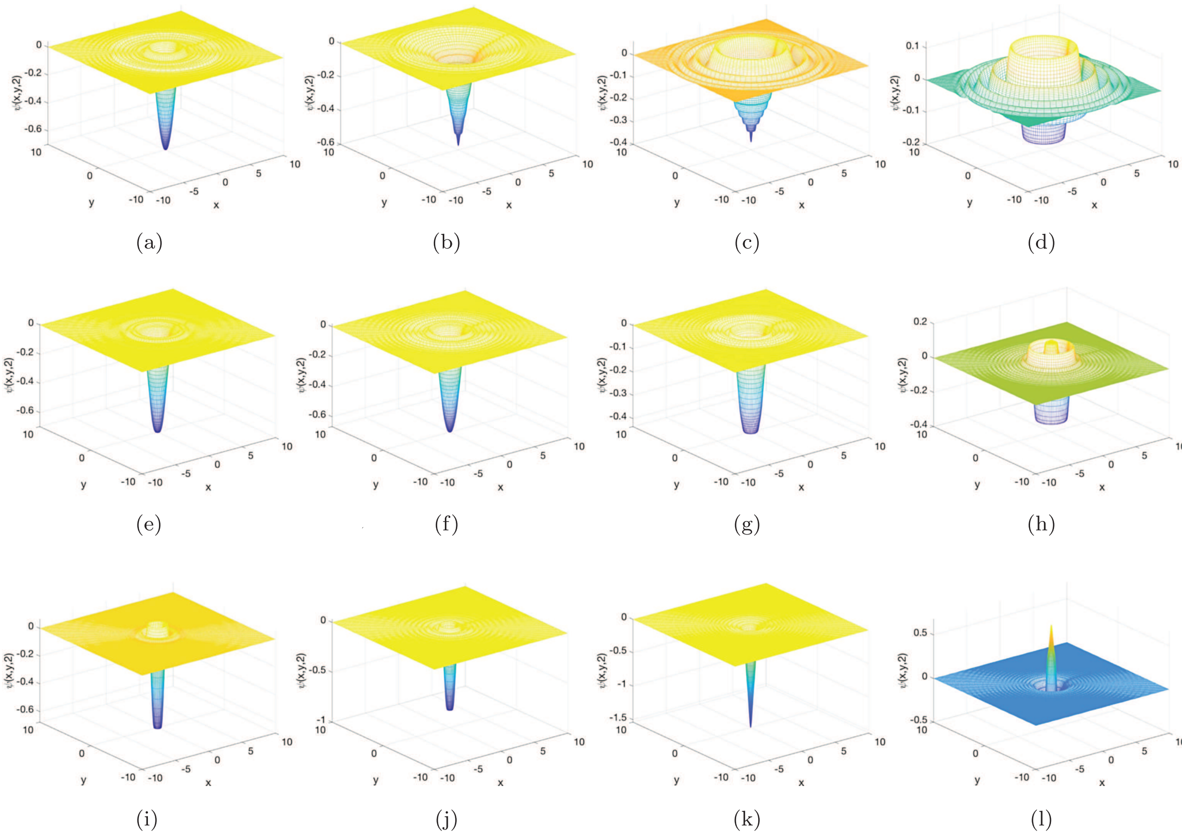


FIGURE 4. The profiles of numerical solution at $t = 2$ with different s, μ. (a) $s = 1$ and $\mu = 1$. (b) $s = 1$ and $\mu = 0.7$. (c) $s = 1$ and $\mu = 0.3$. (d) $s = 1$ and $\mu = -0.3$. (e) $s = 0.7$ and $\mu = 1$. (f) $s = 0.7$ and $\mu = 0.7$. (g) $s = 0.7$ and $\mu = 0.3$. (h) $s = 0.7$ and $\mu = -0.3$. (i) $s = 0.3$ and $\mu = 1$. (j) $s = 0.3$ and $\mu = 0.7$. (k) $s = 0.3$ and $\mu = 0.3$. (l) $s = 0.3$ and $\mu = -0.3$.

4. Müntz-type GHFs with applications to Schrödinger eigenvalue problems

In this section, we introduce the second family of generalised Hermite functions for efficient and spectrally accurate solutions of the Schrödinger eigenvalue problem:

$$\begin{cases} \big[-\frac{1}{2}\Delta + V(\boldsymbol{x})\big]u(\boldsymbol{x}) = \lambda u(\boldsymbol{x}) & \text{in } \mathbb{R}^d, \\ u(\boldsymbol{x}) \to 0 & \text{as } |\boldsymbol{x}| \to \infty, \end{cases} \tag{4.1}$$

where the potential function $V(\boldsymbol{x}) = Z|\boldsymbol{x}|^{2\alpha}$ with α, Z being given constants. It is known that (i) if $\alpha > -1$, all eigenvalues of (4.1) are distinct; (ii) if $\alpha = -1$ or $Z = 0$, the spectrum of the Schrödinger operator $-\frac{1}{2}\Delta + \frac{Z}{|\boldsymbol{x}|^2}$ is a continuous one (*cf.* [15]).

The variational form of (4.1) is to find $\lambda \in \mathbb{R}$ and $u \in H^1(\mathbb{R}^d)\backslash\{0\}$ such that

$$\mathcal{B}(u,v) := \frac{1}{2}(\nabla u, \nabla v)_{\mathbb{R}^d} + Z(|\boldsymbol{x}|^{2\alpha}u, v)_{\mathbb{R}^d} = \lambda(u,v)_{\mathbb{R}^d}, \quad \forall\, v \in H^1(\mathbb{R}^d). \tag{4.2}$$

As shown in Lemma 2.7, the Hermite functions $\{\widehat{H}^{0,n}_{k,\ell}(\boldsymbol{x})\}$ are the eigenfunctions of the Schrödinger operator: $-\Delta + |\boldsymbol{x}|^2$. Here, we intend to explore similar properties for the more general operator by introducing the Müntz-type Hermite functions, and construct efficient and spectrally accurate spectral approximation to (4.2).

4.1. Müntz-type generalised Hermite functions

To solve (4.2) accurately and efficiently, we introduce the following M-GHFs that are orthogonal in the sense of (4.5) below.

Definition 4.1. For $\theta > 0, (\ell, n) \in \Upsilon^d_\infty$ and $k \in \mathbb{N}_0$, the Müntz-type GHFs are defined by

$$\widehat{\mathcal{H}}^{\theta,n}_{k,\ell}(\boldsymbol{x}) = c^{\theta,d}_{k,n}\, L^{(\beta_n)}_k(|\boldsymbol{x}|^{2\theta})\mathrm{e}^{-\frac{|\boldsymbol{x}|^{2\theta}}{2}}\, Y^n_\ell(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^d, \tag{4.3}$$

where

$$c^{\theta,d}_{k,n} = \sqrt{\frac{2\,k!}{\Gamma(k+\beta_n+1)}}, \quad \beta_n = \beta^{\theta,d}_n = \frac{n+d/2-1}{\theta}.$$

It is seen from (2.13) and (4.3) that if $\theta = 1$, it reduces the GHFs $\widehat{H}^{0,n}_{k,\ell}(\boldsymbol{x})$, *i.e.*, $\widehat{\mathcal{H}}^{1,n}_{k,\ell}(\boldsymbol{x}) = \widehat{H}^{0,n}_{k,\ell}(\boldsymbol{x})$. The so-defined Müntz-type GHFs enjoy the following remarkable properties, which are key to the success of the spectral algorithm for (4.2).

Theorem 4.2. *For $\theta > \max(1-d/2, 0)$, $(\ell, n), (\iota, m) \in \Upsilon^d_\infty$ and $k, j \in \mathbb{N}_0$, we have*

$$\big[-\Delta + \theta^2|\boldsymbol{x}|^{4\theta-2}\big]\widehat{\mathcal{H}}^{\theta,n}_{k,\ell}(\boldsymbol{x}) = 2\theta^2(\beta_n+2k+1)\,|\boldsymbol{x}|^{2\theta-2}\widehat{\mathcal{H}}^{\theta,n}_{k,\ell}(\boldsymbol{x}), \tag{4.4}$$

and the orthogonality

$$\big(\nabla\,\widehat{\mathcal{H}}^{\theta,n}_{k,\ell}, \nabla\,\widehat{\mathcal{H}}^{\theta,m}_{j,\iota}\big)_{\mathbb{R}^d} + \theta^2\big(|\boldsymbol{x}|^{4\theta-2}\widehat{\mathcal{H}}^{\theta,n}_{k,\ell}, \widehat{\mathcal{H}}^{\theta,m}_{j,\iota}\big)_{\mathbb{R}^d} = 2\,\theta\,\big(\beta_n+2k+1\big)\delta_{jk}\delta_{mn}\delta_{\ell\iota}. \tag{4.5}$$

Proof. We can derive from (2.3), (2.10), (2.23), (4.3) and the change of variable $\rho = r^\theta$ that

$$\begin{aligned}
&\big[-\Delta + \theta^2 r^{4\theta-2}\big]\widehat{\mathcal{H}}^{\theta,n}_{k,\ell}(\boldsymbol{x})\\
&= c^{\theta,d}_{k,n}\Big(-\frac{1}{r^{d-1}}\partial_r r^{d-1}\partial_r - \frac{1}{r^2}\Delta_{\mathbb{S}^{d-1}} + \theta^2 r^{4\theta-2}\Big)\,[r^n\,L^{(\beta_n)}_k(r^{2\theta})\mathrm{e}^{-\frac{r^{2\theta}}{2}}\,Y^n_\ell(\hat{\boldsymbol{x}})]\\
&= c^{\theta,d}_{k,n}\Big(-\frac{1}{r^{d-1}}\partial_r r^{d-1}\partial_r + \frac{n(n+d-2)}{r^2} + \theta^2 r^{4\theta-2}\Big)\,[r^n\,L^{(\beta_n)}_k(r^{2\theta})\mathrm{e}^{-\frac{r^{2\theta}}{2}}\,Y^n_\ell(\hat{\boldsymbol{x}})]\\
&= \theta^2\rho^{2-\frac{2}{\theta}}\Big(-\frac{1}{\rho^{\frac{d+2\theta-2}{\theta}-1}}\partial_\rho\rho^{\frac{d+2\theta-2}{\theta}-1}\partial_\rho + \frac{\frac{n}{\theta}(\frac{n}{\theta}+\frac{d+2\theta-2}{\theta}-2)}{\rho^2} + \rho^2\Big)\,[\rho^{\frac{n}{\theta}}\,L^{(\beta_n)}_k(\rho^2)\mathrm{e}^{-\frac{\rho^2}{2}}\,Y^n_\ell(\hat{\boldsymbol{x}})]\\
&= \theta^2\rho^{2-\frac{2}{\theta}}\Big(4k + \frac{2n}{\theta} + \frac{d+2\theta-2}{\theta}\Big)\,[\rho^{\frac{n}{\theta}}\,L^{(\beta_n)}_k(\rho^2)\mathrm{e}^{-\frac{\rho^2}{2}}\,Y^n_\ell(\hat{\boldsymbol{x}})]\\
&= 2\theta^2\big(\beta_n+2k+1\big)r^{2\theta-2}[r^n\,L^{(\beta_n)}_k(r^{2\theta})\mathrm{e}^{-\frac{r^{2\theta}}{2}}\,Y^n_\ell(\hat{\boldsymbol{x}})]\\
&= 2\theta^2\big(\beta_n+2k+1\big)|\boldsymbol{x}|^{2\theta-2}\widehat{\mathcal{H}}^{\theta,n}_{k,\ell}(\boldsymbol{x}),
\end{aligned}$$

where we used the identity derived from ([28], Lem. 2.1) with $\alpha = \frac{n+d/2-1}{\theta}$ and $\beta = \alpha + \frac{1-d/2}{\theta}$:

$$\Big[\partial^2_\rho + \frac{\frac{d+2\theta-2}{\theta}-1}{\rho}\partial_\rho - \frac{\frac{n}{\theta}(\frac{n}{\theta}+\frac{d+2\theta-2}{\theta}-2)}{\rho^2} - \rho^2 + 4k + \frac{2n}{\theta} + \frac{d+2\theta-2}{\theta}\Big]\big[\rho^{\frac{n}{\theta}}L^{(\beta_n)}_k(\rho^2)\,\mathrm{e}^{-\frac{\rho^2}{2}}\big] = 0.$$

Next, we prove the orthogonality (4.5). By virtue of (4.4), we have from (4.3) and the change of variable $\rho = r^{2\theta}$ that

$$
\begin{aligned}
&\big(\nabla \widehat{\mathcal{H}}^{\theta,n}_{k,\ell}, \nabla \widehat{\mathcal{H}}^{\theta,m}_{j,\iota}\big)_{\mathbb{R}^d} + \theta^2\big(|\boldsymbol{x}|^{4\theta-2}\, \widehat{\mathcal{H}}^{\theta,n}_{k,\ell}, \widehat{\mathcal{H}}^{\theta,m}_{j,\iota}\big)_{\mathbb{R}^d} \\
&= 2\theta^2(\beta_n + 2k + 1)(c^{\theta,d}_{k,n})^2 \delta_{mn}\delta_{\ell\iota} \int_0^\infty r^{2\theta+2n+d-3} L^{(\beta_n)}_k(r^{2\theta}) L^{(\beta_n)}_j(r^{2\theta}) \mathrm{e}^{-r^{2\theta}}\mathrm{d}r \\
&= \theta(\beta_n + 2k + 1)(c^{\theta,d}_{k,n})^2 \delta_{mn}\delta_{\ell\iota} \int_0^\infty \rho^{\beta_n} L^{(\beta_n)}_k(\rho) L^{(\beta_n)}_j(\rho) \mathrm{e}^{-\rho}\mathrm{d}\rho \\
&= 2\,\theta(\beta_n + 2k + 1)\,\delta_{mn}\delta_{jk}\delta_{\ell\iota}.
\end{aligned}
$$

This completes the proof. □

As a special case of (4.4) (*i.e.*, $\theta = \frac{1}{2}$), we can find the explicit representation of the eigen-pairs of the Schrödinger operator with Coulomb potential: $-\frac{1}{2}\Delta - \frac{|Z|}{|\boldsymbol{x}|}$ in d dimension, where Z is a nonzero constant.

Corollary 4.3. *For any $k \in \mathbb{N}_0$, $(\ell, n) \in \Upsilon^d_\infty$ and $Z \neq 0$, we have*

$$
\Big[-\frac{1}{2}\Delta - \frac{|Z|}{|\boldsymbol{x}|}\Big]\widehat{\mathcal{H}}^{\frac{1}{2},n}_{k,\ell}\Big(\frac{4|Z|\,\boldsymbol{x}}{2n+2k+d-1}\Big) = -\frac{2Z^2}{(2n+2k+d-1)^2}\widehat{\mathcal{H}}^{\frac{1}{2},n}_{k,\ell}\Big(\frac{4|Z|\,\boldsymbol{x}}{2n+2k+d-1}\Big). \tag{4.6}
$$

Proof. Taking $\theta = \frac{1}{2}$ in (4.4) and rearranging the terms, leads to

$$
\Big[-\Delta - \frac{\beta_n + 2k + 1}{2|\boldsymbol{x}|}\Big]\widehat{\mathcal{H}}^{\frac{1}{2},n}_{k,\ell}(\boldsymbol{x}) = -\frac{1}{4}\widehat{\mathcal{H}}^{\frac{1}{2},n}_{k,\ell}(\boldsymbol{x}).
$$

With a rescaling in r direction

$$
\boldsymbol{x} \to \frac{4|Z|\,\boldsymbol{x}}{\beta_n + 2k + 1} = \frac{4|Z|\,\boldsymbol{x}}{2n+2k+d-1},
$$

we can obtain (4.6) immediately. □

The identity in Corollary 4.3 implies that the spectra of the Schrödinger operator with Coulomb potential are given by

$$
\{\lambda_i, u^n_{i,\ell}\} := \Big\{-\frac{2Z^2}{(2i+d-3)^2},\ \widehat{\mathcal{H}}^{\frac{1}{2},n}_{i-n-1,\ell}\Big(\frac{4|Z|\,\boldsymbol{x}}{2i+d-3}\Big)\Big\}, \quad (\ell,n) \in \Upsilon^d_{i-1},\ i \in \mathbb{N}, \tag{4.7}
$$

and the multiplicity of each λ_i is

$$
m^d_i := a^d_0 + a^d_1 + \cdots + a^d_{i-1} = \frac{(i-1)_{d-1} + (i)_{d-1}}{(d-1)!}, \quad d \geqslant 2,
$$

where we recall that a^d_i (defined in (2.6)) is the cardinality of $\Upsilon^d_i \backslash \Upsilon^d_{i-1}$ (defined in (2.9)).

Remark 4.4. The spectrum of the Schrödinger operator with Coulomb potential is of much interest in quantum mechanics and mathematical physics. For example, one can find the spectrum expressions in *e.g.*, ([33], p. 132) and ([16], Thm. 10.10) for $d = 3$ with a different derivation, and the recent work [32] for the asymptotic study of the eigenfunctions. □

Although the orthogonality (4.5) does not imply the orthogonality of each individual term, the stiffness and mass matrices are sparse with finite bandwidth.

Theorem 4.5. *For $\theta > \max(1-d/2, 0)$, $(\ell, n), (\iota, m) \in \Upsilon_\infty^d$ and $k, j \in \mathbb{N}_0$, we have*

$$\big(\nabla \widehat{\mathcal{H}}_{k,\ell}^{\theta,n}, \nabla \widehat{\mathcal{H}}_{j,\iota}^{\theta,m}\big)_{\mathbb{R}^d} = \theta\, \delta_{mn}\delta_{\ell\iota} \times \begin{cases} \beta_n + 2k + 1, & j = k, \\ \sqrt{(k+1)\big(\beta_n + k + 1\big)}, & j = k+1, \\ \sqrt{(j+1)\big(\beta_n + j + 1\big)}, & k = j+1, \\ 0, & \textit{otherwise}, \end{cases} \tag{4.8}$$

and for $n + d/2 + \alpha > 0$,

$$\begin{aligned} \big(|\boldsymbol{x}|^{2\alpha} \widehat{\mathcal{H}}_{k,\ell}^{\theta,n}, \widehat{\mathcal{H}}_{j,\iota}^{\theta,m}\big)_{\mathbb{R}^d} &= \frac{1}{2\theta}\, c_{k,n}^{\theta,d}\, c_{j,n}^{\theta,d}\, \delta_{mn}\, \delta_{\ell\iota} \\ &\times \sum_{p=0}^{\min(k,j)} \frac{\Gamma(k-p+1-\frac{1+\alpha}{\theta})\Gamma(j-p+1-\frac{1+\alpha}{\theta})\Gamma(p+\beta_n+\frac{1+\alpha}{\theta})}{\Gamma^2(1-\frac{1+\alpha}{\theta})\,(k-p)!\,(j-p)!\,p!}. \end{aligned} \tag{4.9}$$

Proof. In view of the definition (4.3), we derive from (2.8), (2.11), (2.22) and the change of variable $\rho = r^{2\theta}$, we derive

$$\begin{aligned} \big(|\boldsymbol{x}|^{2\alpha} \widehat{\mathcal{H}}_{k,\ell}^{\theta,n}, \widehat{\mathcal{H}}_{j,\iota}^{\theta,m}\big)_{\mathbb{R}^d} &= c_{k,n}^{\theta,d} c_{j,n}^{\theta,d} \delta_{mn}\delta_{\ell\iota} \int_0^\infty r^{2n+d-1+2\alpha} L_k^{(\beta_n)}(r^{2\theta}) L_j^{(\beta_n)}(r^{2\theta})\, \mathrm{e}^{-r^{2\theta}}\, \mathrm{d}r \\ &= \frac{1}{2\theta} c_{k,n}^{\theta,d} c_{j,n}^{\theta,d} \delta_{mn}\delta_{\ell\iota} \int_0^\infty \rho^{\frac{n+d/2-1}{\theta} + \frac{\alpha+1-\theta}{\theta}} L_k^{(\beta_n)}(\rho) L_j^{(\beta_n)}(\rho)\, \mathrm{e}^{-\rho} \mathrm{d}\rho \\ &= \frac{1}{2\theta} c_{k,n}^{\theta,d} c_{j,n}^{\theta,d} \delta_{mn}\delta_{\ell\iota} \sum_{p=0}^{k}\sum_{q=0}^{j} \frac{\Gamma(k-p+\frac{\theta-1-\alpha}{\theta})}{\Gamma(\frac{\theta-1-\alpha}{\theta})(k-p)!} \frac{\Gamma(j-q+\frac{\theta-1-\alpha}{\theta})}{\Gamma(\frac{\theta-1-\alpha}{\theta})(j-q)!} \\ &\times \int_0^\infty \rho^{\frac{n+d/2+\alpha-\theta}{\theta}} L_p^{(\frac{n+d/2+\alpha-\theta}{\theta})}(\rho) L_q^{(\frac{n+d/2+\alpha-\theta}{\theta})}(\rho)\, \mathrm{e}^{-\rho} \mathrm{d}\rho \\ &= \frac{c_{k,n}^{\theta,d}\, c_{j,n}^{\theta,d}}{2\theta}\, \delta_{mn}\, \delta_{\ell\iota} \sum_{p=0}^{\min(k,j)} \frac{\Gamma(k-p+\frac{\theta-1-\alpha}{\theta})\Gamma(j-p+\frac{\theta-1-\alpha}{\theta})\Gamma(p+\frac{n+d/2+\alpha}{\theta})}{\Gamma^2(\frac{\theta-1-\alpha}{\theta})\,(k-p)!\,(j-p)!\,p!}, \end{aligned} \tag{4.10}$$

which gives (4.9). In particular, if $\alpha = 2\theta - 1$, we derive from (4.10) that

$$\begin{aligned} \big(|\boldsymbol{x}|^{4\theta-2} \widehat{\mathcal{H}}_{k,\ell}^{\theta,n}, \widehat{\mathcal{H}}_{j,\iota}^{\theta,m}\big)_{\mathbb{R}^d} &= \frac{1}{2\theta} c_{k,n}^{\theta,d} c_{j,n}^{\theta,d} \delta_{mn}\delta_{\ell\iota} \int_0^\infty \rho^{\beta_n+1} L_k^{(\beta_n)}(\rho) L_j^{(\beta_n)}(\rho)\, \mathrm{e}^{-\rho} \mathrm{d}\rho \\ &= \frac{1}{\theta}\, \delta_{mn}\delta_{\ell\iota} \times \begin{cases} \beta_n + 2k + 1, & j = k, \\ -\sqrt{(k+1)\big(\beta_n + k + 1\big)}, & j = k+1, \\ -\sqrt{(j+1)\big(\beta_n + j + 1\big)}, & k = j+1, \\ 0, & \text{otherwise}. \end{cases} \end{aligned} \tag{4.11}$$

Then (4.8) is a direct consequence of (4.5) and (4.11). Note that (4.11) can be also obtained from (4.10) with the understanding $\Gamma(z) = 0$ if z is negative integer. □

4.2. Schrödinger eigenvalue problem with a Coulomb potential

In what follows, we implement the Hermite spectral method for the three-dimensional Schrödinger eigenvalue problem (4.1) with a Coulomb potential $V(\boldsymbol{x}) = \frac{Z}{|\boldsymbol{x}|}$ with $Z < 0$ for the hydrogen atom [41], that is,

$$\Big(-\frac{1}{2}\Delta + \frac{Z}{|\boldsymbol{x}|}\Big) u(\boldsymbol{x}) = \lambda u(\boldsymbol{x}), \quad \boldsymbol{x} \in \mathbb{R}^3. \tag{4.12}$$

Numerical solution of (4.12) poses at least two challenges (i) nonpositive definiteness of the variational form and (ii) the singularity of the Coulomb potential. To overcome these, we shall propose an efficient and accurate spectral method by using the Müntz-type GHFs with a suitable parameter $\theta = \frac{1}{2}$, in light of the Coulomb potential.

Define the approximation space

$$\mathcal{W}_{N,K} = \operatorname{span}\big\{\widehat{\mathcal{H}}^{\frac{1}{2},n}_{k,\ell}(\kappa \boldsymbol{x}):\ 0 \leqslant n \leqslant N,\ 1 \leqslant \ell \leqslant 2n+1,\ 0 \leqslant k \leqslant K,\ k,\ell,n \in \mathbb{N}_0\big\},$$

where a scaling factor $\kappa > 0$ is used to enhance the performance of the spectral approximation as in usual Hermite spectral methods in one dimension (see, *e.g.,* [38, 44]). The spectral approximation scheme for (4.2) is to find $\lambda_{N,K} \in \mathbb{R}$ and $u_{N,K} \in \mathcal{W}_{N,K} \backslash \{0\}$ such that

$$\mathcal{B}(u_{N,K}, v_{N,K}) = \lambda_{N,K}(u_{N,K}, v_{N,K})_{\mathbb{R}^3}, \quad \forall\, v_{N,K} \in \mathcal{W}_{N,K}. \tag{4.13}$$

In real implementation, we write

$$u_{N,K}(\boldsymbol{x}) = \sum_{n=0}^{N} \sum_{\ell=1}^{2n+1} \sum_{k=0}^{K} \hat{u}^n_{k,\ell}\, \widehat{\mathcal{H}}^{\frac{1}{2},n}_{k,\ell}(\kappa \boldsymbol{x}),$$

and denote

$$\hat{\boldsymbol{u}}^n_\ell = \big(\hat{u}^n_{0,\ell}, \hat{u}^n_{1,\ell}, \ldots, \hat{u}^n_{K,\ell}\big)^t, \quad \boldsymbol{u} = \big(\hat{\boldsymbol{u}}^0_1, \hat{\boldsymbol{u}}^1_1, \hat{\boldsymbol{u}}^1_2, \hat{\boldsymbol{u}}^1_3, \cdots, \hat{\boldsymbol{u}}^N_1, \hat{\boldsymbol{u}}^N_2, \cdots, \hat{\boldsymbol{u}}^N_{2N+1}\big)^t. \tag{4.14}$$

With this ordering, we denote the stiffness and the mass matrices by $\boldsymbol{S}$ and $\boldsymbol{M}$, respectively, with the entries given by

$$\begin{aligned}\mathcal{B}(\widehat{\mathcal{H}}^{\frac{1}{2},n}_{k,\ell}(\kappa\cdot), \widehat{\mathcal{H}}^{\frac{1}{2},m}_{j,\iota}(\kappa\cdot)) &= \frac{1}{2\kappa}\Big[(\nabla \widehat{\mathcal{H}}^{\frac{1}{2},n}_{k,\ell}, \nabla \widehat{\mathcal{H}}^{\frac{1}{2},m}_{j,\iota})_{\mathbb{R}^3} + \frac{1}{4}(\widehat{\mathcal{H}}^{\frac{1}{2},n}_{k,\ell}, \widehat{\mathcal{H}}^{\frac{1}{2},m}_{j,\iota})_{\mathbb{R}^3}\Big] \\ &\quad + \frac{Z}{\kappa^2}\big(|\boldsymbol{x}|^{-1}\widehat{\mathcal{H}}^{\frac{1}{2},n}_{k,\ell}, \widehat{\mathcal{H}}^{\frac{1}{2},m}_{j,\iota}\big)_{\mathbb{R}^3} - \frac{1}{8\kappa}\big(\widehat{\mathcal{H}}^{\frac{1}{2},n}_{k,\ell}, \widehat{\mathcal{H}}^{\frac{1}{2},m}_{j,\iota}\big)_{\mathbb{R}^3}, \\ \big(\widehat{\mathcal{H}}^{\frac{1}{2},n}_{k,\ell}(\kappa\cdot), \widehat{\mathcal{H}}^{\frac{1}{2},m}_{j,\iota}(\kappa\cdot)\big)_{\mathbb{R}^3} &= \frac{1}{\kappa^3}\big(\widehat{\mathcal{H}}^{\frac{1}{2},n}_{k,\ell}, \widehat{\mathcal{H}}^{\frac{1}{2},m}_{j,\iota}\big)_{\mathbb{R}^3}.\end{aligned}$$

Owing to (4.5) and (4.11) with $\theta = \frac{1}{2}$, both the stiffness matrix $\boldsymbol{S}$ and the mass matrix $\boldsymbol{M}$ are tridiagonal.

Consequently, the scheme (4.13) has an equivalent form in the following algebraic eigen-system:

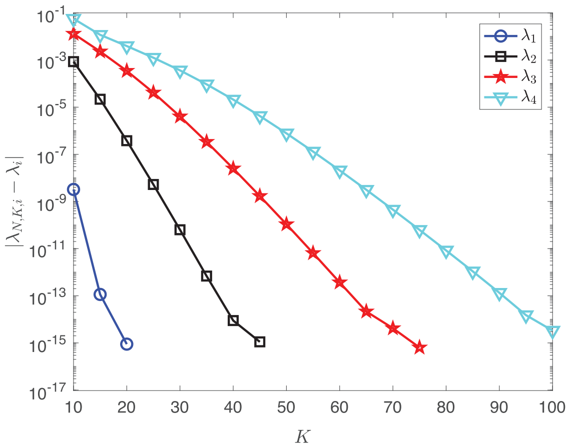
$$\boldsymbol{S}\boldsymbol{u} = \lambda_N \boldsymbol{M}\boldsymbol{u}. \tag{4.15}$$

Interestingly, the matrix $\boldsymbol{S} + \frac{\kappa^2}{8}\boldsymbol{M}$ is diagonal, so we can rewrite (4.15) as

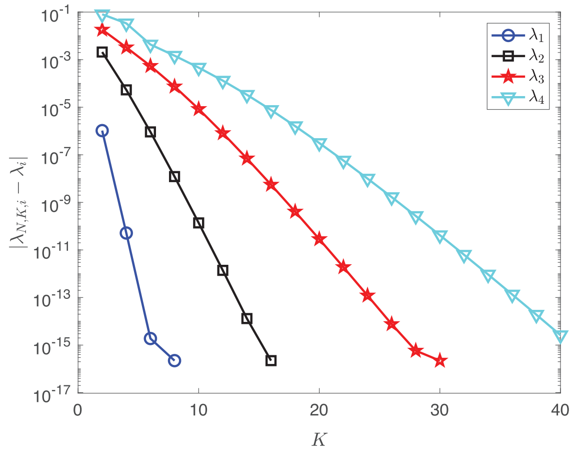
$$\Big(\boldsymbol{S} + \frac{\kappa^2}{8}\boldsymbol{M}\Big)\boldsymbol{u} = \Big(\lambda_N + \frac{\kappa^2}{8}\Big)\boldsymbol{M}\boldsymbol{u},$$

which leads a more efficient implementation.

In Figure 5, we plot the errors between the first 30 (counted by multiplicity) smallest numerical eigenvalues and exact eigenvalues in (4.7) *versus* K for fixed $N = 16$ and two different scaling factors (so that the error of the truncation in angular directions is negligible). Observe that the errors decay exponentially in terms of the cut-off number in the radial direction, along which the eigenfunctions are singular. We also see that the scaling parameter affects the convergence rate as the usual Hermite method (*cf.* [44]).



(a)



(b)

FIGURE 5. The errors of the smallest 4 eigenvalues without counting multiplicities *versus* K for solving (4.12) with $Z=-1$. (a) $N=16$ and $\kappa=4$. (b) $N=16$ and $\kappa=7/4$.

4.3. Schrödinger eigenvalue problem with a fractional power potential

Note that for any given rational number $\frac{q}{p}>-2$ with $p\in\mathbb{N}$ and $q\in\mathbb{Z}$, we can always rewrite it as

$$\frac{q}{p}=\frac{2\nu-2\mu}{\mu+1}\quad\text{with}\quad \mu=2p-1\in\mathbb{N},\;\; \nu=2p+q-1\in\mathbb{N}_0. \tag{4.16}$$

In the sequel, we consider the following Schrödinger equation with a fractional power potential as follows

$$-\frac{1}{2}\Delta u(\boldsymbol{x})+Z|\boldsymbol{x}|^{\frac{2\nu-2\mu}{\mu+1}}u(\boldsymbol{x})=\lambda u(\boldsymbol{x}),\qquad \boldsymbol{x}\in\mathbb{R}^d, \tag{4.17}$$

where $\mu,\nu\in\mathbb{N}_0$. Hereafter, we choose the Müntz-type GHF approximation with $\theta=\frac{1}{\mu+1}$, to account for both the accuracy and efficiency. Accordingly, we define the approximation space

$$\mathcal{W}_{N,K}^{d,\frac{1}{\mu+1}}=\operatorname{span}\big\{\widehat{\mathcal{H}}_{k,\ell}^{\frac{1}{\mu+1},n}(\kappa\boldsymbol{x}):\;0\leqslant n\leqslant N,\;1\leqslant\ell\leqslant a_n^d,\;0\leqslant k\leqslant K,\;k,\ell,n\in\mathbb{N}_0\big\},\quad d\geqslant 2,$$

and for $d=1$, we can always assume μ is odd and then define the approximation space as

$$\mathcal{W}_{N,K}^{1,\frac{1}{\mu+1}}=\operatorname{span}\big\{\widehat{\mathcal{H}}_{k,1}^{\frac{1}{\mu+1},n}(\kappa\boldsymbol{x}):\;\frac{\mu+1}{2}\delta_{n,0}\leqslant k\leqslant K,\;n=0,1\big\},$$

where $\{\widehat{\mathcal{H}}_{k,1}^{\frac{1}{\mu+1},n}\}$ are understood as the Müntz-type GHFs defined through generalized Laguerre polynomials $L_k^{(\beta_0)}$ with the negative integer $\beta_0=-\frac{\mu+1}{2}$ (*cf.* [26]). This turns out important to deal with the strong singularities at the origin to ensure $u(0)=0$ in one dimension.

The generalized Hermite spectral method for (4.2) is to find $\lambda_{N,K}\in\mathbb{R}$ and $u_{N,K}\in\mathcal{W}_{N,K}^{d,\frac{1}{\mu+1}}\backslash\{0\}$ s.t.

$$\mathcal{B}(u_{N,K},v_{N,K})=\lambda_{N,K}(u_{N,K},v_{N,K})_{\mathbb{R}^d},\quad\forall\, v_{N,K}\in\mathcal{W}_{N,K}^{d,\frac{1}{\mu+1}}. \tag{4.18}$$

In the implementation, we write

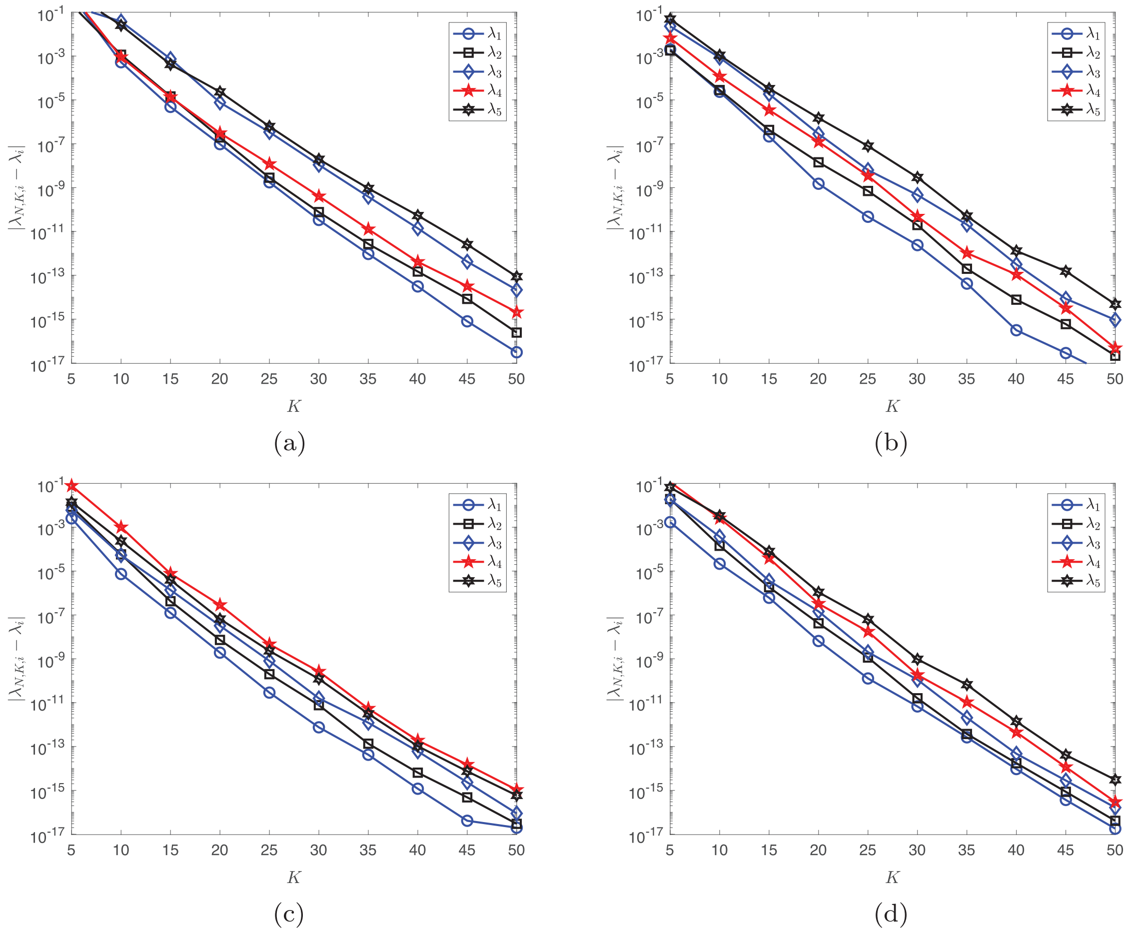


FIGURE 6. The errors of the smallest 5 eigenvalues without counting multiplicities *versus* K for solving (4.17) with $N = 10$. (a) $d = 4$, $Z = 1$, $\mu = 3$, $\nu = 5$ and $\kappa = 500$. (b) $d = 3$, $Z = 1$, $\mu = 1$, $\nu = 2$ and $\kappa = 2$. (c) $d = 2$, $Z = 3$, $\mu = 1$, $\nu = 4$ and $\kappa = 10$. (d) $d = 1$, $Z = -3$, $\mu = 3$, $\nu = 2$ and $\kappa = 70$.

$$u_{N,K}(\boldsymbol{x}) = \sum_{n=0}^{N} \sum_{\ell=1}^{a_n^d} \sum_{k=0}^{K} \hat{u}_{k,\ell}^n \, \widehat{\mathcal{H}}_{k,\ell}^{\frac{1}{\mu+1},n}(\kappa \boldsymbol{x}),$$

and denote

$$\hat{\boldsymbol{u}}_\ell^n = \big(\hat{u}_{0,\ell}^n, \hat{u}_{1,\ell}^n, \ldots, \hat{u}_{K,\ell}^n\big)^t, \quad \boldsymbol{u} = \big(\hat{\boldsymbol{u}}_1^0, \hat{\boldsymbol{u}}_2^0, \cdots, \hat{\boldsymbol{u}}_{a_0^d}^0, \hat{\boldsymbol{u}}_1^1, \hat{\boldsymbol{u}}_2^1, \cdots, \hat{\boldsymbol{u}}_{a_1^d}^1, \cdots, \hat{\boldsymbol{u}}_1^N, \hat{\boldsymbol{u}}_2^N, \cdots, \hat{\boldsymbol{u}}_{a_N^d}^N\big)^t. \tag{4.19}$$

The corresponding algebraic eigen-system of (4.18) is

$$\boldsymbol{S}\boldsymbol{u} = \lambda_N \boldsymbol{M}\boldsymbol{u}. \tag{4.20}$$

In view of orthogonality (4.8) and (4.9), we find that for any $q \in \mathbb{N}_0$,

$$\big(|\boldsymbol{x}|^{\frac{2q-2\mu}{\mu+1}} \widehat{\mathcal{H}}_{k,\ell}^{\frac{1}{\mu+1},n}(\kappa\cdot), \widehat{\mathcal{H}}_{j,\iota}^{\frac{1}{\mu+1},m}(\kappa\cdot)\big)_{\mathbb{R}^d} = \kappa^{-d}\big(\widehat{\mathcal{H}}_{k,\ell}^{\frac{1}{\mu+1},n}, \widehat{\mathcal{H}}_{j,\iota}^{\frac{1}{\mu+1},m}\big)_{\mathbb{R}^d}$$

$$= \frac{\mu+1}{2}\kappa^{-d}\, c_{k,n}^{\frac{1}{\mu+1},d}\, c_{j,n}^{\frac{1}{\mu+1},d}\, \delta_{mn}\,\delta_{\ell\iota} \sum_{p=\max(j-q,k-q,0)}^{\min(k,j)} \frac{\Gamma(k-p-q)\Gamma(j-p-q)\Gamma(p+\beta_n+q+1)}{\Gamma^2(-q)\,(k-p)!\,(j-p)!\,p!}$$

$$= \frac{\mu+1}{2}\kappa^{-d}\, c_{k,n}^{\frac{1}{\mu+1},d}\, c_{j,n}^{\frac{1}{\mu+1},d}\, \delta_{mn}\,\delta_{\ell\iota} \sum_{p=\max(j-q,k-q,0)}^{\min(k,j)} \frac{(-q)_{k-p}(-q)_{j-p}\Gamma(p+\beta_n+q+1)}{(k-p)!\,(j-p)!\,p!}.$$

Furthermore, one has

$$\begin{aligned}\mathcal{B}(\widehat{\mathcal{H}}_{k,\ell}^{\frac{1}{\mu+1},n}(\kappa\cdot),\widehat{\mathcal{H}}_{j,\iota}^{\frac{1}{\mu+1},m}(\kappa\cdot)) &= \frac{1}{2}\,\kappa^{2-d}(\nabla\,\widehat{\mathcal{H}}_{k,\ell}^{\frac{1}{\mu+1},n},\nabla\widehat{\mathcal{H}}_{j,\iota}^{\frac{1}{\mu+1},m})_{\mathbb{R}^d}\\ &\quad + Z\,\kappa^{-\frac{2\nu-2\mu}{\mu+1}-d}(|\boldsymbol{x}|^{\frac{2\nu-2\mu}{\mu+1}}\,\widehat{\mathcal{H}}_{k,\ell}^{\frac{1}{\mu+1},n},\widehat{\mathcal{H}}_{j,\iota}^{\frac{1}{\mu+1},m})_{\mathbb{R}^d}.\end{aligned}$$

These indicate that the stiffness matrix $\boldsymbol{S}$ is a sparse banded matrix with a bandwidth $\max(\nu,1)$, and the mass matrix $\boldsymbol{M}$ is also a sparse banded matrix with a bandwidth μ.

In the numerical tests, we fix $N=10$, choose different scaling factor κ and test for different Z, μ,ν and dimensions. Numerical errors between the smallest eigenvalues without counting multiplicities and the reference eigenvalues (obtained by the scheme with large N and K) are depicted in Figure 6. Exponential orders of convergence are clearly observed in all cases, which demonstrate the effectiveness of the new Hermite spectral method.

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References

[1] M.S. Agranovich, Sobolev Spaces, their Generalizations and Elliptic Problems in Smooth and Lipschitz domains. *Springer Monographs in Mathematics*. Springer, Cham (2015).

[2] G.E. Andrews, R. Askey and R. Roy, Special Functions. Cambridge (1999).

[3] R. Askey, Orthogonal Polynomials and Special Functions. Society for Industrial and Applied Mathematics (1975).

[4] W. Bao, H. Li and J. Shen, A generalized Laguerre-Fourier-Hermite pseudospectral method for computing the dynamics of rotating Bose-Einstein condensates. *SIAM J. Sci. Comput.* **31** (2009) 3685–3711.

[5] W. Bao, X. Ruan, J. Shen and C. Sheng, Fundamental gaps of the fractional Schrödinger operator. *Commun. Math. Sci.* **17** (2019) 447–471.

[6] W. Bao, L. Chen, X. Jiang and Y. Ma, A Jacobi spectral method for computing eigenvalue gaps and their distribution statistics of the fractional Schrödinger operator. *J. Comput. Phys.* **421** (2020) 109733.

[7] P. Borwein, T. Erdélyi and J. Zhang, Müntz systems and orthogonal Müntz-Legendre polynomials. *Trans. Amer. Math. Soc.* **342** (1994) 523–542.

[8] D. Burnett, The distribution of molecular velocities and the mean motion in a non-uniform gas. *Proc. London Math. Soc.* **40** (1936) 382–435.

[9] Z. Cai, Y. Fan and Y. Wang, Burnett spectral method for the spatially homogeneous Boltzmann equation. *Comput. & Fluids* **200** (2020) 104456.

[10] T. Chihara, *Generalized Hermite polynomials*. Ph.D. thesis, Purdue University (1955).

[11] T. Chihara, An Introduction to Orthogonal Polynomials. New York (1978).

[12] F. Dai and Y. Xu, Approximation Theory and Harmonic Analysis on Spheres and Balls. Springer-Verlag (2013).

[13] E. Di Nezza, G. Palatucci and E. Valdinoci, Hitchhiker's guide to the fractional Sobolev spaces. *Bull. Sci. Math.* **136** (2012) 521–573.

[14] C.F. Dunkl and Y. Xu, Orthogonal Polynomials of Several Variables, 2nd edition. vol. 155, Cambridge University Press, Cambridge (2014).

[15] Z.J. Duoandikoetxea, Fourier Analysis, vol. 29, American Mathematical Society (2001).

[16] T. Gerald, Mathematical Methods in Quantum Mechanics with Applications to Schrödinger Operators, 2nd edition. *Graduate Studies in Mathematics*. Vol. 157. American Mathematical Society, Providence, RI (2014).

[17] I.S. Gradshteyn and I.M. Ryzhik, Table of Integrals, Series, and Products, 8th edition. Elsevier/Academic Press, Amsterdam (2015).

[18] G.A. Hagedorn, Semiclassical quantum mechanics. I. The $h \to 0$ limit for coherent states. *Comm. Math. Phys.* **71** (1980) 77–93.

[19] D. Hou and C. Xu, A fractional spectral method with applications to some singular problems. *Adv. Comput. Math.* **43** (2017) 911–944.

[20] Z. Hu and Z. Cai, Burnett spectral method for high-speed rarefied gas flows. *SIAM J. Sci. Comput.* **42** (2020) 1193–1226.

[21] L. Klebanov, *Approximation of PDEs with Underlying Continuity Equations.* Ph.D. thesis, Technische Universität, München (2015).

[22] N. Laskin, Fractional quantum mechanics and Lévy path integrals. *Phys. Lett. A* **268** (2000) 298–305.

[23] C. Lasser and S. Troppmann, Hagedorn wavepackets in time-frequency and phase space. *J. Fourier Anal. Appl.* **20** (2014) 679–714.

[24] C. Lasser and C. Lubich, Computing quantum dynamics in the semiclassical regime. *Acta Numer.* **29** (2020) 229–401.

[25] N.N. Lebedev, Special Functions and their Applications, edited by Richard A. Silverman. Prentice-Hall, Inc., Englewood Cliffs, N.J. (1965).

[26] F. Liu, Z. Wang and H. Li, A fully diagonalized spectral method using generalized Laguerre functions on the half line. *Adv. Comput. Math.* **43** (2017) 1227–1259.

[27] C. Lubich, From Quantum to Classical Molecular Dynamics: Reduced Models and Numerical Analysis. European Mathematical Society, Zürich (2008).

[28] S. Ma, H. Li and Z. Zhang, Novel spectral methods for Schrödinger equations with an inverse square potential on the whole space. *Discrete Contin. Dyn. Syst. Ser. B* **24** (2019) 1589–1615.

[29] Z. Mao and J. Shen, Hermite spectral methods for fractional PDEs in unbounded domains. *SIAM J. Sci. Comput.* **39** (2017) A1928–A1950.

[30] M. Masjed-Jamei and W. Koepf, Two classes of special functions using Fourier transforms of generalized ultraspherical and generalized Hermite polynomials. *Proc. Amer. Math. Soc.* **140** (2012) 2053–2063.

[31] C.H. Müntz. Über den Approximationssatz von Weierstrass, in H.A. Schwarz's Festschrift, Berlin (1914) 303–312.

[32] V.I. Osherov and V.G. Ushakov. Analytical solutions of the Schrödinger equation for a hydrogen atom in a uniform electric field. *Phys. Rev. A.* **95** (2017) 023419.

[33] L. Pauling and E.B. Wilson, Introduction to Quantum Mechanics with Applications to Chemistry. McGraw-Hill (1935).

[34] L.P. Pitaevskii and S. Stringari, Bose-Einstein Condensation. Oxford University Press, Oxford (2003).

[35] M. Rosenblum, Generalized Hermite polynomials and the Bose-like oscillator calculus. Nonselfadjoint operators and related topics. *Oper. Theory Adv. Appl.* **73** (1994) 369–396.

[36] M. Rösler, Generalized Hermite polynomials and the heat equation for Dunkl operators. *Comm. Math. Phys.* **192** (1998) 519–542.

[37] T.S. Shao, T.C. Chen and R.M. Frank, Tables of zeros and Gaussian weights of certain associated Laguerre polynomials and the related generalized Hermite polynomials. *Math. Comp.* **18** (1964) 598–616.

[38] J. Shen, T. Tang and L.-L. Wang, Spectral Methods: Algorithms, Analysis and Applications. Springer (2011).

[39] J. Shen and Y. Wang, Müntz-Galerkin methods and applications to mixed Dirichlet-Neumann boundary value problems. *SIAM J. Sci. Comput.* **38** (2016) A2357–A2381.

[40] C. Sheng, J. Shen, T. Tang, L.-L. Wang and H. Yuan, Fast Fourier-like mapped Chebyshev spectral-Galerkin methods for PDEs with integral fractional Laplacian in unbounded domains. *SIAM J. Numer. Anal.* **58** (2020) 2435–2464.

[41] E. Schrödinger, Quantisierung als Eigenwertproblem. *Annalen der Physik* **384** (1926) 361–377.

[42] G. Strang and G. Fix, An Analysis of the Finite Element Method. *prentice-Hall Series in Automatic Computation*, Prentice-Hall Inc., Englewood Cliffs, N.J. (1973).

[43] G. Szegö, Orthogonal Polynomials. American Mathematical Society, Providence (1939).

[44] T. Tang, The Hermite spectral method for Gaussian-type functions. *SIAM J. Sci. Comput.* **14** (1993) 594–606.

[45] T. Tang, H. Yuan and T. Zhou, Hermite spectral collocation methods for fractional PDEs in unbounded domains. *Commun. Comput. Phys.* **24** (2018) 1143–1168.

[46] A. Yurova, *Generalized Anisotropic Hermite Functions and their Applications*. Ph.D. thesis, Technische Universität, München (2020).

[47] Y. Zhang, X. Liu, M. Belić, *et al.*, Propagation dynamics of a light beam in a fractional Schrödinger equation. *Phys. Rev. Lett.* **115** (2015) 180403.