GENERALISED HERMITE FUNCTIONS AND THEIR APPLICATIONS IN
SPECTRAL APPROXIMATIONS

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ABSTRACT. In 1939, G. Szegö first introduced a family of generalised Hermite polynomials (GHPs) as a generalisation of usual Hermite polynomials, which are orthogonal with respect to the weight function $|x|^{2\mu}e^{-x^2}$, $\mu > -\frac{1}{2}$ on the whole line. Since then, there have been a few works on the study of their properties, but no any on their applications to numerical solutions of partial differential equations (PDEs). The main purposes of this paper are twofold. The first is to construct the generalised Hermite polynomials and generalised Hermite functions (GHFs) in arbitrary $d$ dimensions, which are orthogonal with respect to $|x|^{2\mu}e^{-|x|^2}$ and $|x|^{2\mu}$ in $\mathbb{R}^d$, respectively. We then define a family of adjoint generalised Hermite functions ($A$-GHFs) upon GHFs, which has two appealing properties: (i) the Fourier transform maps $A$-GHF to the corresponding GHF; and (ii) $A$-GHFs are orthogonal with respect to the inner product $\langle u, v \rangle_{\mathcal{H}^r(\mathbb{R})} = \langle (-\Delta)^{\frac{r}{2}} u, (-\Delta)^{\frac{r}{2}} v \rangle_{L^2(\mathbb{R})}$ associated with the integral fractional Laplacian. The second purpose is to explore their applications in spectral approximations of PDEs. As a remarkable consequence of the fractional Sobolev-type orthogonality, the spectral-Galerkin method using $A$-GHFs as basis functions leads to an identity stiffness matrix for the integral fractional Laplacian operator $(-\Delta)^s$, which is known to be notoriously difficult and expensive to discretise. Indeed, the $A$-GHFs provide an optimal basis for Hermite approximation of $(-\Delta)^s$ in $\mathbb{R}^d$. As a by-product, the $A$-GHFs with integer parameter $s$ can significantly improve the existing Hermite spectral-Galerkin algorithms for PDEs with usual Laplacian. We also conduct rigorous error analysis of approximation by GHFs and of the optimal spectral method for fractional PDEs in $\mathbb{R}^d$. The second application is to solve the eigenvalue problem of the Schrödinger operator involving a general fractional power potential. Following the same spirit, we further introduce a Müntz-type GHFs that are orthogonal with respect to an inner product associated with the Schrödinger operator. Using the new basis, the Hermite spectral-Galerkin algorithm can fully diagonalise certain Schrödinger operators, and leads to sparse mass and stiffness matrices with finite bandwidth. Moreover, the Müntz-type GHF expansion can fit the singularity of the eigenfunctions. It is confident that this work can significantly enrich both the theory and applications of spectral methods for unbounded domains.

1. INTRODUCTION

In the seminal monograph \cite{19} (P. 371) (1939), Szegö first introduced 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 polynomials (GHPs)), through an explicit second-order differential equation in an exercise problem. The GHPs defined therein are orthogonal with respect to the weight function $|x|^{2\mu}e^{-x^2}$. Chihara perhaps was among the first who systematically studied the properties of the GHPs, and the associated generalised

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Hermite functions (GHFs): \( \hat{H}_n^{(\mu)}(x) := e^{-x^2/2}H_n^{(\mu)}(x) \) (orthogonal with respect to the weight function \(|x|^{2\mu}\)), in his PhD thesis \[12\] entitled as “Generalised Hermite Polynomials” (1955). Later, some standard properties were collected in his book \[13\] (2011). Whereas the usual Hermite polynomials/functions are well-studied and developed in spectral approximations (see, e.g., \[24, 33, 7, 52, 26, 11, 10\] and the reference therein), the works on this generalised family are limited to the study of the properties or further generalisations (see, e.g., \[12, 40, 41, 6, 35\] and a few references therein). Indeed, to the best of our knowledge, the generalised Hermite spectral methods in both theory and applications are still under-explored, and worthy of deep investigation.

It is known that the usual Hermite functions \( \{\hat{H}_n^{(0)}\} \) are eigenfunctions of the Fourier transform (see, e.g., \[19\]). This appealing property turned out crucial for algorithm developments in many scenarios. For example, He, Li and Shen \[27\] considered the numerical solutions of unbounded rough surface scattering problems, where the reduction of the unbounded domain via the global Dirichlet-to-Neumann operator involving the Fourier transform of the unknown field, and the use of Hermite functions could decouple the problems. More recently, the Hermite spectral-Galerkin and collocation methods proposed in \[34, 51\] for the integral fractional Laplacian in unbounded domains essentially relied on the Fourier transform invariant properties of usual Hermite functions. However, this merit does not carry over to the GHFs with \( \mu \neq 0 \). It is quite common that the orthogonal polynomials are transformed into other special functions by the Fourier transforms. Indeed, the explicit formula for the Fourier transform of \( |x|^{2\mu}\hat{H}_n^{(\mu)}(x) \) with \( \mu, \nu > -\frac{1}{2} \) are given in \[35\] (2.34) in terms of the Kummer hypergeometric functions \( _1F_1(\cdot) \).

Chihara's thesis \[12, P. 53\] obtained the formula for the Fourier transform of \( e^{x^2}\hat{H}_n^{(\mu)}(x) \) (i.e., the over-scaled GHF: \( e^{-x^2/2}\hat{H}_n^{(\mu)}(x) \)):

\[
\int_{\mathbb{R}} e^{-x^2} H_n^{(\mu)}(x) e^{-i2\xi x} \, dx = \sqrt{\pi}^{\mu} \left[ \left( \frac{n}{2} - \mu + 1 \right) \xi \right]^{-\frac{1}{2}} e^{-\frac{n}{2}} _1F_1 \left( -\left\lfloor \frac{n}{2} \right\rfloor - \left\lfloor \frac{n}{2} \right\rfloor - \mu + 1, \xi^2 \right). \tag{1.1}
\]

In particular, if \( \mu = 0 \), it reduces to the formula for the usual over-scaled Hermite function (cf. \[37, 18.18.23\]):

\[
\int_{\mathbb{R}} e^{-x^2} H_n^{(0)}(x) e^{-i\xi x} \, dx = \sqrt{\pi} (-i\xi)^n e^{-\frac{\xi^2}{4}}, \tag{1.2}
\]

which played an important role in \[51\] for computing the spectral collocation differentiation matrices of the fractional Laplacian.

The main objectives of this paper are twofold. The first is to introduce a family of adjoint generalised Hermite functions (A-GHFs), denoted by \( \widetilde{H}_n^{(\mu)}(x) \), through a judicious linear combination of the Hermite functions \( \{\tilde{H}_j^{(0)}(x)\}_{j=0}^n \), which satisfy the following two notable properties (see Theorem 3.1):

(i) The Fourier transform maps the A-GHF to the GHF:

\[
\mathcal{F}[\tilde{H}_n^{(\mu)}](\xi) = (-i)^n \tilde{H}_n^{(\mu)}(\xi), \quad \mu > -\frac{1}{2}. \tag{1.3}
\]

In other words, the Fourier transforms of the A-GHFs are orthogonal with respect to the weight function \(|\xi|^{2\mu}\) in \(\mathbb{R}\).

(ii) The A-GHFs are orthogonal with respect to the inner product that induces the so-called Gagliardo semi-norm of \(H^s(\mathbb{R})\), that is,

\[
[\tilde{H}_n^{(s)}, \tilde{H}_m^{(s)}]_{H^s(\mathbb{R})} = (\langle (\Delta) \tilde{H}_n^{(s)}, (\Delta) \tilde{H}_m^{(s)} \rangle_{H^s(\mathbb{R})}) = 0, \quad \text{if} \ m \neq n, \tag{1.4}
\]

where the integral fractional Laplacian is defined as \[2.3\]. As an important application, the spectral-Galerkin method using the A-GHFs as basis functions, leads to an identity matrix for the integral fractional operator. It is known that the fractional operator is much more expensive and difficult to deal with, due to the nonlocal nature and the involved singular kernel (see \[20\].

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for a very recent review). As such, the use of the new basis, the Hermite spectral algorithm is optimal. More importantly, all these are valid for multiple dimensions.

The second purpose of this paper is to introduce the GHPs/GHFs and their adjoint cousins in arbitrary dimension, which preserve the attractive properties (i)-(ii), and to explore their applications as well. More precisely, based upon the relation between the GHPs and generalised Laguerre polynomials (expressed in terms of confluent hypergeometric functions, see [12]), the $d$-dimensional GHPs/GHFs are constructed through a “warped” tensorial product of the generalised Laguerre polynomials (in radial direction) with the spherical harmonics (in angular direction) (cf. [15]). We term this non-standard tensorial structure as a “warped” tensor for the reason that the parameters of the generalised Laguerre polynomials depend on the degree parameter of the spherical harmonics. This situation is reminiscent to the orthogonal polynomials on triangles/hexahedra (cf. [17, 30]) constructed from Jacobi polynomials through the Duffy transformation [18]. By construction, the $d$-dimensional GHPs and GHFs are orthogonal with respect to $|x|^{2\mu}e^{-|x|^2}$ and $|x|^{2\mu}$ with $\mu > -\frac{1}{2}$, respectively. Correspondingly, we define the adjoint GHFs satisfying the properties (1.3)-(1.4) in $d$-dimensions. We shall demonstrate through two examples of applications: (a) fractional PDE with integral fractional Laplacian, and (b) eigenvalue problem involving Schrödinger operator with a general fractional power potential, that the A-GHFs and their interesting variants are natural and optimal basis functions for the Hermite spectral methods for such problems. Moreover, we also conduct rigorous error analysis of spectral approximation by GHFs and of the proposed methods for fractional Laplacian. Several points are worthy of highlighting.

1. The family of A-GHFs with integer $\mu$ is of independent interest. For example, the Hermite spectral-Galerkin methods using the A-GHFs with $\mu = 1$ as basis function can lead to identity stiffness matrix for the usual Laplacian, which is not possible for the usual Hermite spectral algorithms studied in literature. This is very similar to development of the optimal spectral algorithms using generalised Jacobi polynomials for boundary value problems in bounded domains (cf. [25]).

2. The three-dimensional GHPs with a special parameter $\mu = 0$ and an appropriate scaling reduce to the Burnett polynomials [8] (1936), which are mutually orthogonal with respect to the Maxwellian $\mathcal{M}(x) = (2\pi)^{-3/2}e^{-|x|^2}$, and are useful in solving kinetic equations (see, e.g., [9] and the references therein).

3. Following the same spirit of diagonalising the fractional Laplacian operator, we further generalise this notion and introduce a Müntz-type GHFs tailored to the Schrödinger operator with a general fractional power potential. The new GHF-spectral-Galerkin approximation can not only diagonalise this operator (which is not feasible for other Hermite functions), but also fit the singularity of the eigenfunctions leading to spectrally accurate algorithms. More specifically, with properly chosen parameters, our Müntz-type GHFs recover the hydrogen-like wave functions, i.e., eigenfunctions of the Schrödinger operator with a Coulomb potential.

The rest of the paper is organised as follows. In Section 2, we make necessary preparations by introducing some notation, spaces of functions and the spherical harmonics. We then study the one-dimensional GHPs/GHFs, and estimate the weighted $L^2$-errors of the related orthogonal projections. We introduce in Section 4 the multi-dimensional GHPs/GHFs and their adjoint counterparts, and present some remarkable properties indispensable for developing optimal Hermite spectral algorithms. In Section 5 we develop and analyse optimal Hermite spectral-Galerkin methods for PDEs with integral fractional Laplacian in $\mathbb{R}^d$. In Section 6 we introduce a more general family of Müntz-type GHFs and apply it to the eigenvalue problem of the Schrödinger operator with a general fractional power potential. We conclude the paper in the final section.

2. Preliminaries

In this section, we make necessary preparations for the forthcoming exposition and discussions. We first introduce some notation, and spaces of functions related to the integral fractional Laplacian. We then
recall some relevant properties of the spherical harmonics in $d$ dimensions, which will be an indispensable building block for the multi-dimensional GHPs and GHFs.

2.1. Notation and spaces of functions. Let $\mathbb{N}$ be the set of positive integers and $\mathbb{N}_0 := \{0\} \cup \mathbb{N}$. For $\alpha \in \mathbb{R}$ and $-\alpha \notin \mathbb{N}_0$, the rising factorial in the Pochhammer symbol is defined as

$$(\alpha)_0 := 1, \quad (\alpha)_k = \alpha(\alpha+1)(\alpha+2) \cdots (\alpha+k-1) = \frac{\Gamma(\alpha+k)}{\Gamma(\alpha)}, \quad k \geq 1. \quad (2.1)$$

Let $\mathbb{R}^d$ be the $d$-dimensional Euclidean space. For any $x, y \in \mathbb{R}^d$, we define the inner product and norm of $\mathbb{R}^d$ as $\langle x, y \rangle := \sum_{i=1}^d x_i y_i$, and $|x| := \sqrt{\langle x, x \rangle}$, respectively. Denote the unit vector along $x$ by $\hat{x} = x/|x|$. Consider functions in the Schwartz class $\mathcal{S}(\mathbb{R}^d)$. For any $u \in \mathcal{S}(\mathbb{R}^d)$, its Fourier transform and inverse Fourier transform are given by

$$\hat{u}(\xi) := \mathcal{F}[u](\xi) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} u(x) e^{-i\langle\xi, x\rangle} \, dx, \quad \mathcal{F}^{-1}[\hat{u}](x) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \hat{u}(\xi) e^{i\langle\xi, x\rangle} \, d\xi.$$

For $s > 0$, the fractional Laplacian of $u \in \mathcal{S}(\mathbb{R}^d)$ can be naturally defined as a pseudodifferential operator characterised by the Fourier transform:

$$(-\Delta)^s u(x) = \mathcal{F}^{-1}\left[[|\xi|^{2s}] \mathcal{F}[u](\xi)\right](x). \quad (2.2)$$

The fractional Laplacian can be equivalently defined by means of the following point-wise formula (cf. [10] Prop. 3.3): for any $u \in \mathcal{S}(\mathbb{R}^d)$ and $s \in (0, 1)$,

$$(-\Delta)^s u(x) = C_{d, s} \, \text{p.v.} \int_{\mathbb{R}^d} \frac{u(x) - u(y)}{|x - y|^{d+2s}} \, dy, \quad x \in \mathbb{R}^d, \quad (2.3)$$

where “p.v.” stands for the principle value and the normalization constant

$$C_{d, s} := \left( \int_{\mathbb{R}^d} \frac{1 - \cos \xi_1}{|\xi|^{d+2s}} \, d\xi \right)^{-1} = \frac{2^{2s} \, s \Gamma(s + d/2)}{\pi^{d/2} \Gamma(1 - s)}.$$

For real $s \geq 0$, we define the fractional Sobolev space (cf. [10] P. 530):

$$H^s(\mathbb{R}^d) = \left\{ u \in L^2(\mathbb{R}^d) : \|u\|_{H^s(\mathbb{R}^d)}^2 = \int_{\mathbb{R}^d} (1 + |\xi|^{2s}) |\mathcal{F}[u](\xi)|^2 \, d\xi < +\infty \right\}, \quad (2.4)$$

and an analogous definition for the case $s < 0$ is to set

$$H^s(\mathbb{R}^d) = \left\{ u \in \mathcal{S}'(\mathbb{R}^d) : \|u\|_{H^s(\mathbb{R}^d)}^2 = \int_{\mathbb{R}^d} (1 + |\xi|^{2s}) |\mathcal{F}[u](\xi)|^2 \, d\xi < +\infty \right\},$$

although in this case the space $H^s(\mathbb{R}^d)$ is not a subset of $L^2(\mathbb{R}^d)$.

According to [10] Prop. 3.4, we know that for $s \in (0, 1)$, the space $H^s(\mathbb{R}^d)$ can also be characterised by the fractional Laplacian defined in (2.3), equipped with the norm

$$\|u\|_{H^s(\mathbb{R}^d)} = \left( \|u\|_{L^2(\mathbb{R}^d)}^2 + \|(-\Delta)^{s/2} u\|_{L^2(\mathbb{R}^d)}^2 \right)^{\frac{1}{2}},$$

where $|u|_{H^s(\mathbb{R}^d)}$ is the so-called Gagliardo semi-norm of $u$, given by

$$|u|_{H^s(\mathbb{R}^d)} := \left( \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{|u(x) - u(y)|^2}{|x - y|^{d+2s}} \, dx \, dy \right)^{\frac{1}{2}}. \quad (2.5)$$

Indeed, by [10] Prop. 3.6, we have that for $s \in (0, 1)$,

$$|u|_{H^s(\mathbb{R}^d)}^2 = 2C_{d, s}^{-1} \|(-\Delta)^{s/2} u\|_{L^2(\mathbb{R}^d)}^2. \quad (2.6)$$

We have the following important space interpolation property (cf. [2] Ch. 1), which will be used for the error analysis later on.
Lemma 2.1. For real $r_0, r_1 \geq 0$, let $r = (1 - \theta)r_0 + \theta r_1$ with $\theta \in [0, 1]$. Then for any $u \in H^{r_0}(\mathbb{R}^d) \cap H^{r_1}(\mathbb{R}^d)$, we have
\[
\|u\|_{H^r(\mathbb{R}^d)} \leq \|u\|_{H^{r_0}(\mathbb{R}^d)}^{1-\theta} \|u\|_{H^{r_1}(\mathbb{R}^d)}^\theta.
\]
In particular, for $s \in [0,1]$, we have
\[
\|u\|_{H^s(\mathbb{R}^d)} \leq \|u\|_{L^2(\mathbb{R}^d)}^{1-s} \|u\|_{H^1(\mathbb{R}^d)}^s.
\]

2.2. Spherical harmonics. We next introduce the $d$-dimensional spherical harmonics, upon which the $d$-dimensional generalised Hermite polynomials/functions are built. Here, we follow the same definitions and settings as in the book [14]. Let $\mathcal{P}_n^d$ be the space of all real homogeneous polynomials of degree $n$ in $d$ variables:
\[
\mathcal{P}_n^d = \text{span}\{x^k = x_1^{k_1} x_2^{k_2} \cdots x_d^{k_d} : k_1 + k_2 + \cdots + k_d = n\}.
\]
That is, a homogeneous polynomial $P(x)$ of degree $n$ is a linear combination of monomials of degree $n$. As an important subspace of $\mathcal{P}_n^d$, the space of all real harmonic polynomials of degree $n$ is defined as
\[
\mathcal{H}_n^d := \{ P \in \mathcal{P}_n^d : \Delta P(x) = 0 \}.
\]
It is known that
\[
\dim(\mathcal{P}_n^d) = \binom{n + d - 1}{n}, \quad a_n^d := \dim(\mathcal{H}_n^d) = \binom{n + d - 1}{n} - \binom{n + d - 3}{n - 2},
\]
where it is understood that for $n = 0,1$, the value of the second binomial coefficient is zero (cf. [14 (1.1.5)]). In other words, for $d = 1$, the harmonic polynomials are spanned by \{1, x\}.

We introduce the $d$-dimensional spherical coordinates:
\[
x_1 = r \cos \theta_1; \quad x_2 = r \sin \theta_1 \cos \theta_2; \quad \ldots; \quad x_{d-1} = r \sin \theta_1 \cdots \sin \theta_{d-2} \cos \theta_{d-1};
\]
\[
x_d = r \sin \theta_1 \cdots \sin \theta_{d-1} \sin \theta_d, \quad r &= |x|, \quad \theta_1, \ldots, \theta_{d-2} \in [0, \pi], \quad \theta_{d-1} \in [0, 2\pi],
\]
and the spherical volume element is
\[
dx = r^{d-1} \sin^{d-2}(\theta_1) \sin^{d-3}(\theta_2) \cdots \sin(\theta_{d-2}) \, dr \, d\theta_1 \ldots d\theta_{d-1} := r^{d-1} dr \, d\sigma(\hat{x}).
\]
In spherical coordinates, the Laplace operator takes the form
\[
\Delta = \nabla^2 + \frac{d - 1}{r} \nabla_r + \frac{1}{r^2} \Delta_{S^{d-1}},
\]
where $\Delta_{S^{d-1}}$ is the Laplace-Beltrami operator on the unit sphere $S^{d-1} := \{x \in \mathbb{R}^d : r = |x| = 1\}$.

The $d$-dimensional spherical harmonics are the restrictions of harmonic polynomials in $\mathcal{H}_n^d$ to $S^{d-1}$. For clarity, we denote by $\mathcal{H}_n^d|_{S^{d-1}}$ the space of all spherical harmonics of degree $n$. It is important to take note of the correspondence between a harmonic polynomial and the related spherical harmonic function (cf. [14 Ch. 1]): for any $Y(x) \in \mathcal{H}_n^d$,
\[
Y(x) = |x|^n Y(|x|/|x|) = r^n Y(\hat{x}), \quad \hat{x} \in S^{d-1},
\]
and then $Y(\hat{x}) \in \mathcal{H}_n^d|_{S^{d-1}}$. It is also noteworthy that $Y(x)$ is a homogeneous polynomial in $\mathbb{R}^d$, while $Y(\hat{x})$ is a non-polynomial function on the unit sphere.

Define the inner product on $S^{d-1}$ as
\[
\langle f, g \rangle_{S^{d-1}} := \int_{S^{d-1}} f(\hat{x}) g(\hat{x}) \, d\sigma(\hat{x}),
\]
under which the spherical harmonics of different degree are orthogonal to each other (cf. [14 Thm. 1.1.2]), i.e., $\mathcal{H}_m^d|_{S^{d-1}} \perp \mathcal{H}_m^d|_{S^{d-1}}$ for $m \neq n$. For $n \in \mathbb{N}_0$, let $\{Y_{\ell}^n : 1 \leq \ell \leq a_n^d\}$ be the (real) spherical harmonic basis of $\mathcal{H}_n^d|_{S^{d-1}}$, which are normalised so that
\[
\langle Y_{\ell}^n, Y_{\ell'}^m \rangle_{S^{d-1}} = \delta_{nm} \delta_{\ell \ell'}, \quad 1 \leq \ell \leq a_n^d, \quad 1 \leq \ell' \leq a_n^d, \quad m \geq 0, \quad n \geq 0.
\]
The basis functions $Y_{\ell}^n(\hat{x})$ are also called Laplace spherical harmonic functions of degree $n$ and order $\ell$, as they are eigenfunctions
\[
\Delta_{S^{d-1}} Y_{\ell}^n(\hat{x}) = -n(n + d - 2) Y_{\ell}^n(\hat{x}).
\]
Remark 2.1. The representations of the spherical harmonic basis functions in terms of the Gegenbauer polynomials in the spherical coordinates are given in [14 Thm. 1.5.1]. Below, we list them for \( d = 1, 2, 3 \).

(i) For \( d = 1 \), we note from (2.11) that \( a_0^0 = a_1^1 = 1 \) and \( a_n^1 = 0 \) for \( n \geq 2 \), so there exist only two orthonormal polynomials: \( Y_1^0(x) = \frac{1}{\sqrt{2}} \) and \( Y_1^1(x) = \frac{x}{\sqrt{2}} \).

(ii) For \( d = 2 \), the dimensionality of the space \( \mathcal{H}_n^2 \) is \( a_2^n = 2 - \delta_{n0} \) and the orthogonal basis of \( \mathcal{H}_n^2 \) can be given by the real and imaginary parts of \( (x_1 + ix_2)^n \). In polar coordinates \( x = (r \cos \theta, r \sin \theta)^t \in \mathbb{R}^2 \), they simply take the form

\[
Y_1^0(x) = \frac{1}{\sqrt{2\pi}}, \quad Y_1^1(x) = \frac{r}{\sqrt{\pi}} \cos n\theta, \quad Y_2^n(x) = \frac{r^n}{\sqrt{\pi}} \sin n\theta, \quad n \geq 1.
\]  

(2.18)

(iii) For \( d = 3 \), the dimensionality of \( \mathcal{H}_n^3 \) is \( a_3^n = 2n + 1 \). The orthonormal basis in the spherical coordinates \( x = (r \sin \theta \cos \phi, r \sin \theta \sin \phi, r \cos \theta)^t \) takes the form

\[
Y_1^0(x) = \frac{1}{\sqrt{8\pi}} P_n^{(0,0)}(\cos \theta), \quad Y_2^1(x) = \frac{r^n}{2^{1/2} \sqrt{\pi}} (\sin \theta)^l P_n^{(l,l)}(\cos \theta) \cos(l\phi),
\]

\[
Y_{2l+1}^n(x) = \frac{r^n}{2^{l+1/2} \sqrt{\pi}} (\sin \theta)^l P_n^{(l,l)}(\cos \theta) \sin(l\phi), \quad 1 \leq l \leq n,
\]

where \( P_n^{(l,l)}(x) \) are the Gegenbauer polynomials.

3. Generalised Hermite polynomials & functions in one dimension

In this section, we first recall some relevant properties of the one-dimensional GHPs and GHFs. We then construct the adjoint GHFs, and show that it is an optimal basis for spectral approximation of fractional and usual Laplacian. We also provide error estimates for approximation by the GHP/GHF expansions. Although some properties are reducible from the \( d \)-dimensional results in the next section, we feel compelled to consider the one-dimensional case separately for its independence interest in e.g., methods based on multi-dimensional tensorial GHPs/GHFs, and for the clarity of presentation and paving the way for the discussions of the much more involved multi-dimensional case.

3.1. Generalised Hermite polynomials/functions. The generalised Hermite polynomials were first introduced by Szegő in [39 P. 380] in an exercise problem.

Problem 25 Szegő in [39]: Assume \( \mu > -\frac{1}{2} \) and let \( H_n^{(\mu)}(x) \) denote the orthogonal polynomials corresponding to the weight function \( |x|^{2\mu} e^{-x^2} \) in \( \mathbb{R} = (-\infty, \infty) \). Then the following differential equations are satisfied:

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

and

\[
z'' + \left\{ 2n + 2\mu + 1 - x^2 + \frac{(-1)^n \mu - \mu^2}{x^2} \right\} z = 0; \quad z = e^{-x^2/2} x^\mu H_n^{(\mu)}(x).
\]

Remark 3.1. Since the coefficient of (3.2) is an even function of \( x \), both \( z(x) \) and \( z(-x) \) satisfy the same equation. Accordingly, \( z = e^{-x^2/2} x^\mu H_n^{(\mu)}(x) \) is (3.2) should be understood as \( z = e^{-x^2} |x|^\mu H_n^{(\mu)}(x) \).

Throughout the paper, we adopt the normalisation (the leading coefficient of \( H_n^{(\mu)}(x) \) is \( 2^n \)), and review some relevant properties in Chihara [12][13]. We have the orthogonality:

\[
\int_{\mathbb{R}} H_m^{(\mu)}(x) H_n^{(\mu)}(x) |x|^{2\mu} e^{-x^2} \, dx = \gamma_n^{(\mu)} \delta_{mn},
\]

where \( \delta_{mn} \) is the Kronecker symbol and

\[
\gamma_n^{(\mu)} = 2^n \left[ \frac{n}{2} \right] ! \Gamma \left( \frac{n + 1}{2} \right) + \mu + \frac{1}{2}.
\]

(3.3)

(3.4)
with \([x]\) being the greatest integer function. When \(\mu = 0\), the GHPs reduce to the usual Hermite polynomials: \(H_{n}(x) := H_{n}^{(0)}(x)\). Correspondingly, the orthogonality \((3.3), (3.4)\) becomes

\[
\int_{\mathbb{R}} H_{n}(x)H_{m}(x)e^{-x^{2}}dx = \gamma_{n}\delta_{nm}, \quad \gamma_{n} = \sqrt{\pi}2^{n}n!.
\]  

(3.5)

The GHPs can be expressed in terms of generalised Laguerre polynomials:

\[
H_{n}^{(\mu)}(x) = \begin{cases} 
(-1)^{\frac{n}{2}}2^{n}\left(\frac{n}{2}\right)!L_{\frac{n}{2}}^{(\mu-1/2)}(x^{2}), & n \text{ even}, \\
(-1)^{\frac{n-1}{2}}2^{n}\left(\frac{n-1}{2}\right)!xL_{\frac{n-1}{2}}^{(\mu+1/2)}(x^{2}), & n \text{ odd}, 
\end{cases}
\]

(3.6)

where for \(\alpha > -1\), the generalised Laguerre polynomials are orthogonal

\[
\int_{0}^{\infty}L_{k}^{(\alpha)}(z)L_{j}^{(\alpha)}(z)z^{\alpha}e^{-z}dz = \frac{\Gamma(k+\alpha+1)}{k!}\delta_{kj}, \quad k, j \in \mathbb{N}_{0}.
\]

(3.7)

The GHPs satisfy the three-term recurrence relation:

\[
H_{n+1}^{(\mu)}(x) = 2xH_{n}^{(\mu)}(x) - 2(n+\theta_{n})H_{n-1}^{(\mu)}(x), \quad n \geq 1; \quad H_{0}^{(\mu)}(x) = 1, \quad H_{1}^{(\mu)}(x) = 2x,
\]

(3.8)

where \(\theta_{n}\) is defined in \((3.11)\).

The GHPs with different parameters can be transformed from one to the other (cf. \[12, P. 46\]).

**Proposition 3.1.** (see \[12, (12.6)\]). For \(\mu, \nu > -\frac{1}{2}\), there holds

\[
H_{n}^{(\mu)}(x) = \sum_{j+n, \text{even}}^{n} \mu C_{j}^{n} H_{j}^{(\nu)}(x),
\]

(3.9)

where the connection coefficients for even \(j + n\) are given by

\[
\mu C_{j}^{n} = \frac{(-4)^{\frac{n-j}{2}}\Gamma([\frac{j}{2}]+1)\Gamma([\frac{n-j}{2}] + \mu - \nu)}{\Gamma(\mu - \nu)\Gamma([\frac{j}{2}]+1)\Gamma([\frac{n-j}{2}] + 1)}.
\]

(10.10)

**Remark 3.2.** As \(\Gamma(0) = \infty\), we have \(\mu C_{j}^{k} = \delta_{kj}\) for \(\mu = \nu\).

For \(\mu > -\frac{1}{2}\), we define the GHF of degree \(n\) with parameter \(\mu\) by

\[
\hat{H}_{n}^{(\mu)}(x) := \sqrt{1/\gamma_{n}^{(\mu)}}e^{-\frac{x^{2}}{2}}H_{n}^{(\mu)}(x), \quad n \geq 0, \quad x \in \mathbb{R},
\]

(3.11)

where \(\gamma_{n}^{(\mu)}\) be the same as \((3.4)\). It is evident that by \((3.3)\), we have the orthogonality:

\[
\int_{\mathbb{R}} \hat{H}_{l}^{(\mu)}(x)\hat{H}_{n}^{(\mu)}(x)|x|^{2\mu}dx = \delta_{ln}.
\]

(3.12)

In particular, for \(\mu = 0\), we denote \(\hat{H}_{n}(x) = \hat{H}_{n}^{(0)}(x)\) the usual Hermite functions such that

\[
\int_{\mathbb{R}} \hat{H}_{l}(x)\hat{H}_{n}(x)dx = \delta_{ln}.
\]

(3.13)

The GHFs can be computed efficiently in a stable manner by using the following three-term recurrence relation derived from \((3.8)\) and \((3.11)\):

\[
\hat{H}_{n+1}^{(\mu)}(x) = a_{n}^{(\mu)}x\hat{H}_{n}^{(\mu)}(x) - c_{n}^{(\mu)}\hat{H}_{n-1}^{(\mu)}(x), \quad n \geq 1,
\]

\[
\hat{H}_{0}^{(\mu)}(x) = \sqrt{1/\Gamma(\mu + 1/2)}e^{-\frac{x^{2}}{2}}, \quad \hat{H}_{1}^{(\mu)}(x) = \sqrt{1/\Gamma(\mu + 3/2)}x e^{-\frac{x^{2}}{2}},
\]

(3.14)

where

\[
a_{n}^{(\mu)} = \sqrt{\frac{2}{n + 1 + 2\mu - \theta_{n}}}, \quad c_{n}^{(\mu)} = \frac{n + \theta_{n}}{\sqrt{(n + \theta_{n}/(2\mu))(n + 2\mu + 1 - \theta_{n}/(2\mu))}}.
\]

As a direct consequence of Proposition \[3.1\] and \([3.11]\), we have the following transformation between GHFs with different parameters, which plays a very important role in our algorithm development.
Proposition 3.2. For any $\mu, \nu > -\frac{1}{2}$, there holds
\[ \hat{H}^{(\mu)}_n(x) = \sum_{j+n \text{ even}} \mu^j \hat{C}^n_j \hat{H}^{(\nu)}_j(x), \tag{3.15} \]
where for even $j + n$, the connection coefficients are given by
\[ \mu^j \hat{C}^n_j = \frac{(-1)^{\frac{n-j}{2}} \Gamma((\frac{n}{2} + 1) + \frac{j}{2})}{\Gamma((\frac{n}{2} - 1) + \frac{j}{2})} \].

3.2. Adjoint generalised Hermite functions. In what follows, we introduce a new family of orthogonal functions by an appropriate linear combination of Hermite functions, and show that this system enjoys the appealing properties highlighted in (1.3) - (1.4).

Definition 3.1. (Adjoint GHFs). For $\mu > -\frac{1}{2}$, we define the adjoint generalised Hermite function (A-GHF) of degree $n$ and with parameter $\mu$ as
\[ \tilde{H}^{(\mu)}_n(x) = \sum_{j+n \text{ even}} (-1)^{\frac{n-j}{2}} \mu^j \hat{C}^n_j \hat{H}_j(x), \quad x \in \mathbb{R}, \tag{3.17} \]
where the connection coefficients $\{\hat{C}^n_j\}$ are given by (3.16) with $\nu = 0$.

Note that for $\mu = 0$, we have $\tilde{H}^{(0)}_n(x) = \hat{H}_n(x)$ (as $\hat{C}^n_j = \delta_{jn}$), that is, the adjoint of the usual Hermite function is itself. Moreover, we observe from (3.15) that the GHF can be expressed as
\[ \hat{H}^{(\mu)}_n(x) = \sum_{j+n \text{ even}} \hat{C}^n_j \hat{H}_j(x), \quad x \in \mathbb{R}, \tag{3.18} \]
so the adjoint pair $\{\hat{H}^{(\mu)}_n, \tilde{H}^{(\mu)}_n\}$ is intimately related, where in (3.17)-(3.18), the connection coefficients only have some sign difference. More importantly, we have the following interwoven connections through Fourier transforms.

Theorem 3.1. For $\mu > -\frac{1}{2}$, the pair of GHFs satisfies
\[ \mathcal{F}[\tilde{H}^{(\mu)}_n](\xi) = (-i)^n \hat{H}^{(\mu)}_n(\xi), \quad \mathcal{F}^{-1}[\tilde{H}^{(\mu)}_n](x) = i^n \tilde{H}^{(\mu)}_n(x), \] and for $s > 0$,
\[ \mathcal{F}[-(\Delta)^s \tilde{H}^{(\mu)}_n](\xi) = (-i)^n \xi^{2s} \tilde{H}^{(\mu)}_n(\xi). \tag{3.20} \]
Moreover, the adjoint GHFs are orthonormal in the sense that
\[ (-(\Delta)^s \tilde{H}^{(\mu)}_n, -(\Delta)^s \tilde{H}^{(\mu)}_m)_\mathbb{R} = \delta_{mn}. \tag{3.21} \]

Proof. Since the usual Hermite functions are eigenfunctions of the Fourier integral operator (see, e.g., [19]):
\[ \mathcal{F}[\hat{H}_j](\xi) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{H}_j(x)e^{-ix\xi}dx = (-i)^j \hat{H}_j(\xi), \tag{3.22} \]
we obtain from (3.17) and (3.18) readily that
\[ \mathcal{F}[\tilde{H}^{(\mu)}_n](\xi) = \sum_{j+n \text{ even}} (-1)^{\frac{n-j}{2}} \hat{C}^n_j \mathcal{F}[\hat{H}^{(\mu)}_n](\xi) = \sum_{j+n \text{ even}} (-1)^{\frac{n-j}{2}} (-i)^j \hat{C}^n_j \hat{H}_j(x) \]
\[ = (-i)^n \sum_{j+n \text{ even}} \hat{C}^n_j \hat{H}_j(x) = (-i)^n \tilde{H}^{(\mu)}_n(x). \tag{3.23} \]
Here, we used the factor \((-i)^j = (-i)^n(-i)^{2-n} = (-i)^{n}(-i)^{2-n}\) for even \(j \neq n\). It is evident that the second identity in (3.19) follows from the first identity. The relation (3.20) is a direct consequence of (3.19) and the definition of Fractional Laplacian.

Finally, using the Parseval’s identity and (3.20), we obtain from the orthogonality (3.12) that

\[
((\Delta)^{\frac{s}{2}}\tilde{H}_n^{(s)}; (\Delta)^{\frac{s}{2}}\tilde{H}_m^{(s)})_R = \left(\mathcal{F}[(\Delta)^{\frac{s}{2}}\tilde{H}_n^{(s)}], \mathcal{F}[(\Delta)^{\frac{s}{2}}\tilde{H}_m^{(s)}]\right)_R = (-i)^{n-m}\delta_{mn} = \delta_{mn}.
\]

This ends the proof. \(\square\)

As a direct application, the remarkable orthogonality (3.21) of adjoint GHFs can lead to optimal Hermite spectral-Galerkin algorithm for the integral fractional Laplacian. More importantly, the construction is also available for multiple dimensional case, which shall elaborate on in Section 4, and whose error estimates for approximation by GHP/GHF expansions are rendered by using appropriate designed basis functions.

Note that (3.21) is even of interest, since this can at least improve the existing Hermite spectral algorithms (see, e.g., [24, 33, 44]). The key to efficiency is to render the matrix of the leading operator diagonal by using generalised Jacobi polynomials on a finite interval (cf. [25, 43]), where the key to efficiency is to determine the stiffness matrix is identity. This is reminiscent to the optimal spectral-Galerkin algorithms using generalised Jacobi polynomials on a finite interval (cf. [25, 43]), where the key to efficiency is to determine the leading operator diagonal by using appropriate designed basis functions.

### 3.3. Error estimates for approximation by GHP/GHF expansions.

In what follows, we derive some approximation results on the weighted \(L^2\)-type orthogonal projections.

Denote \(\chi^{(\mu)}(x) = x^{2\mu}e^{-x^2}\). Consider the \(L^2_{\chi^{(\mu)}}\)-orthogonal projection \(\Pi^{(\mu)}_N : L^2_{\chi^{(\mu)}}(\mathbb{R}) \rightarrow \mathcal{P}_N\), defined by

\[
(u - \Pi^{(\mu)}_N u, v)_{\chi^{(\mu)}} = 0, \quad \forall v \in \mathcal{P}_N,
\]

or equivalently, we can write

\[
\Pi^{(\mu)}_N u(x) = \sum_{n=0}^{N} \tilde{u}_n H_n^{(\mu)}(x) = \sum_{k=0}^{\left\lfloor \frac{\mu}{2} \right\rfloor} \tilde{u}_{2k} H_{2k}^{(\mu)}(x) + \sum_{k=0}^{\left\lfloor \frac{\mu}{2} \right\rfloor} \tilde{u}_{2k+1} H_{2k+1}^{(\mu)}(x),
\]

with

\[
\tilde{u}_n = \frac{1}{\gamma_n^{(\mu)}}\int_{\mathbb{R}} u(x)H_n^{(\mu)}(x)\chi^{(\mu)}(x)dx.
\]

Denote \(\omega^{(\mu)}(x) = x^{2\mu}\). Then, for any \(u \in L^2_{\omega^{(\mu)}}(\mathbb{R})\), we have \(ue^{\frac{x^2}{2}} \in L^2_{\chi^{(\mu)}}(\mathbb{R})\), and define

\[
\tilde{\Pi}^{(\mu)}_N u := e^{-\frac{x^2}{2}}\Pi^{(\mu)}_N (ue^{\frac{x^2}{2}}) \in \mathcal{V}_N,
\]

which turns out to be the \(L^2_{\omega^{(\mu)}}\)-orthogonal projection, as

\[
(u - \tilde{\Pi}^{(\mu)}_N u, v)_{\omega^{(\mu)}} = (ue^{\frac{x^2}{2}} - \Pi^{(\mu)}_N (ue^{\frac{x^2}{2}}), ve^{\frac{x^2}{2}})_{\chi^{(\mu)}} = 0, \quad \forall v \in \mathcal{V}_N.
\]

Following the analysis framework in [43] for orthogonal polynomial approximations (including Legendre, Chebyshev, Jacobi, Laguerre and usual Hermite polynomials), we need to explore the orthogonality of the derivatives of the polynomials, which actually induces the weighted spaces and leads to
optimal estimates. To this end, we recall the derivative relation of GHPs (cf. [12, P. 42]):
\[ \partial_x H_n^{(\mu)}(x) = 2nH_{n-1}^{(\mu)}(x) + 2(n-1)\theta_n x^{-1}H_{n-2}^{(\mu)}(x), \quad n \geq 1, \]
where \( \theta_{2k} = 0 \) and \( \theta_{2k+1} = 2\mu \) as in (3.32). Observe that the derivative relation becomes “simple” only when \( \mu = 0 \) and \( n = 2k + 1 \). That is, for \( \mu = 0 \), we have
\[ \partial_x H_n(x) = 2nH_{n-1}(x), \quad n \geq 1, \]
and for \( \mu > -\frac{1}{2} \),
\[ \partial_x H_n^{(\mu)}(x) = 4kH_n^{(\mu)}(x), \quad k \geq 1. \]
It is seen from (3.31) and (3.13) that \( \{\partial_x H_n\} \) are also orthogonal in \( L^2(\mathbb{R}) \) with \( \chi(x) = e^{-x^2} \). This attractive property plays an essential role in Hermite approximation (cf. [13, Ch. 7]). However, it is not available for the GHPs with \( \mu \neq 0 \).

Next, we introduce a modified derivative operator and show that the orthogonality in this setting. For this purpose, we decompose a function on \( \mathbb{R} \) into even and odd parts as
\[ u(x) = \frac{u(x) + u(-x)}{2} + \frac{u(x) - u(-x)}{2} = u_e(x) + u_o(x), \quad x \in \mathbb{R}. \]

Assuming that it is differentiable, we then define the new derivative operator:
\[ D_x u = \partial_x u_e + \partial_x \left( \frac{u_o}{2x} \right). \]

Note that if \( u \) is an odd (resp. even) function, then \( D_x u = \partial_x (u/(2x)) \) (resp. \( D_x u = \partial_x u \)). It is clear that by (3.34), \( D_x u \) is an odd function. The modified higher order derivative of general \( u \) simply takes the form
\[ D_x^2 u = D_x \{ D_x u \} = \partial_x \left\{ \frac{D_x u}{2x} \right\}, \quad D_x^2 u = \partial_x \left\{ \frac{1}{2x} \partial_x \left\{ \frac{D_x u}{2x} \right\} \right\}, \]
and likewise, we can define \( D_x^l u \) for \( l \geq 4 \).

**Lemma 3.1.** For \( \mu > -\frac{1}{2} \), the GHPs satisfy
\[ D_x^m H_{2k}^{(\mu)}(x) = d_k^m H_{2k-2m+1}^{(\mu+m-1)}(x), \quad D_x^m H_{2k+1}^{(\mu)}(x) = d_k^m H_{2k-2m+1}^{(\mu+m)}(x), \quad k \geq m, \]
for \( k \geq m \), where
\[ d_k^m = \frac{4^m k!}{(k-m)!}. \]

**Proof.** Recall the recurrence relation (cf. [12, P. 609]):
\[ 2xH_{2k}^{(\mu+1)}(x) = H_{2k+1}^{(\mu)}(x), \quad k \geq 0; \]
which, together with (3.32), implies
\[ D_x H_{2k+1}^{(\mu)}(x) = \partial_x \left\{ \frac{1}{2x} H_{2k+1}^{(\mu)}(x) \right\} = \partial_x H_{2k+1}^{(\mu+1)}(x) = 4kH_{2k-1}^{(\mu+1)}(x). \]
Thus, by (3.36) and (3.39),
\[ D_x^2 H_{2k+1}^{(\mu)}(x) = 4kD_x H_{2k-1}^{(\mu+1)}(x) = 4^2 k(k-1)H_{2k-3}^{(\mu+2)}(x). \]
Using this relation repeatedly yields the second identity in (3.36).

We now turn to the derivation of the first identity. For \( m = 1 \), it coincides with (3.32), so by (3.39),
\[ D_x^2 H_{2k}^{(\mu)}(x) = 4kD_x H_{2k-1}^{(\mu)}(x) = 4k\partial_x \left\{ \frac{1}{2x} H_{2k-1}^{(\mu)}(x) \right\} = 4^2 k(k-1)H_{2k-3}^{(\mu+1)}(x). \]
We can derive the first identity in (3.36) by taking the modified derivative repeatedly. \( \square \)
To characterise the space of functions, we introduce for any \( m \geq 1 \),
\[
\mathcal{B}^m_\mu(\mathbb{R}) := \left\{ u : u \in L^2_{\chi(\mu)}(\mathbb{R}), \; D_x^l u_e \in L^2_{\chi(\mu-l)}(\mathbb{R}), \; D_x^l u_o \in L^2_{\chi(\mu+l)}(\mathbb{R}), \; 1 \leq l \leq m \right\},
\]
equipped with the norm and semi-norm
\[
\| u \|_{\mathcal{B}^m_\mu(\mathbb{R})} = \left( \| u \|_{\chi(\mu)}^2 + \sum_{l=1}^{m} \left( \| D_x^l u_e \|_{\chi(\mu-l)}^2 + \| D_x^l u_o \|_{\chi(\mu+l)}^2 \right) \right)^{\frac{1}{2}},
\]
\[
| u |_{\mathcal{B}^m_\mu(\mathbb{R})} = \left( \| D_x^m u_e \|_{\chi(\mu+m)}^2 + \| D_x^m u_o \|_{\chi(\mu+m)}^2 \right)^{\frac{1}{2}}, \quad m \geq 1.
\]

For \( m = 0 \), we define \( \mathcal{B}^0_\mu(\mathbb{R}) = \mathcal{L}^2_{\chi(\mu)}(\mathbb{R}) \).

**Theorem 3.2.** For any \( u \in \mathcal{B}^m_\mu(\mathbb{R}) \) with \( \mu > -\frac{1}{2}, \mu \neq 0 \) and integer \( 0 \leq m \leq \left\lfloor \frac{N+1}{2} \right\rfloor \), we have that
\[
\| \Pi^0_N u - u \|_{\chi(\mu)} \leq \frac{| u |_{\mathcal{B}^m_\mu(\mathbb{R})}}{\sqrt{\left( \left\lfloor \frac{N+1}{2} \right\rfloor - m + 1 \right) m}}. \quad (3.42)
\]

On the other hand, if \( u e^{\frac{z^2}{2}} \in \mathcal{B}^m_\mu(\mathbb{R}) \), with \( \mu > -\frac{1}{2}, \mu \neq 0 \) and with integer \( 0 \leq m \leq \left\lfloor \frac{N+1}{2} \right\rfloor \), then
\[
\| \tilde{\Pi}^0_N u - u \|_{\chi(\mu)} \leq \frac{| u e^{\frac{z^2}{2}} |_{\mathcal{B}^m_\mu(\mathbb{R})}}{\sqrt{\left( \left\lfloor \frac{N+1}{2} \right\rfloor - m + 1 \right) m}}. \quad (3.43)
\]

**Proof.** We only need to prove the case \( m \geq 1 \), as \( m = 0 \) is obvious. For simplicity, we first assume that \( N \) is odd. It is clear that by (3.27) and (3.33),
\[
\| \Pi^0_N u - u \|_{\chi(\mu)}^2 = \| \Pi^0_N u_o - u_o \|_{\chi(\mu)}^2 + \| \Pi^0_N u_e - u_e \|_{\chi(\mu)}^2. \quad (3.44)
\]

We now deal with the first term. By Lemma 3.1 and (3.3), we have the orthogonality
\[
\int_{\mathbb{R}} D_x^m H_{2k}^{(\mu)}(x) D_x^m H_{2l}^{(\mu)}(x) \chi_{\chi(\mu+m-1)}(x) \, dx = h_{2k,m}^{(\mu)} \delta_{k,l}, \quad (3.45)
\]
where for \( k \geq m \),
\[
h_{2k,m}^{(\mu)} = \left( d_k^{(m)} \right) \gamma_{2k-2m+1}^{(\mu+m-1)} = \frac{2^{4k+2} \Gamma(k+\mu+\frac{1}{2})(k)!}{(k-m)!}. \quad (3.46)
\]
Thus, by the Parseval’s identity, we have
\[
\| D_x^m u_e \|_{\chi(\mu+m-1)}^2 = \sum_{k=m}^{\infty} h_{2k,m}^{(\mu)} | \tilde{u}_{2k} |^2.
\]

In view of (3.45), we obtain from (3.4) and (3.46) that for \( m \geq 1 \),
\[
\| \Pi^0_N u_e - u_e \|_{\chi(\mu)}^2 = \sum_{k=m}^{\infty} \frac{\gamma_{2k}^{(\mu)} | \tilde{u}_{2k} |^2}{\gamma_{2k-2m+1}^{(\mu+m-1)}} \leq \max_{k \geq \frac{N+1}{2}} \left\{ \frac{\gamma_{2k}^{(\mu)}}{h_{2k,m}^{(\mu)}} \right\} \sum_{k=m}^{\infty} h_{2k,m}^{(\mu)} | \tilde{u}_{2k} |^2
\]
\[
\leq \frac{\gamma_{\frac{N+1}{2}}^{(\mu)}}{h_{N+1,m}^{(\mu)}} \| D_x^m u_e \|_{\chi(\mu+m-1)}^2 \leq \frac{\left( \frac{N+1}{2} - m + 1 \right)!}{2^2 (\frac{N+1}{2})!} \| D_x^m u_e \|_{\chi(\mu+m-1)}^2. \quad (3.47)
\]

Similarly, by Lemma 3.1 and (3.3), we have the orthogonality
\[
\int_{\mathbb{R}} D_x^m H_{2k+1}^{(\mu)}(x) D_x^m H_{2l+1}^{(\mu)}(x) \chi_{\chi(\mu+m)}(x) \, dx = h_{2k+1,m}^{(\mu)} \delta_{k,l}, \quad (3.48)
\]
where for \( k \geq m \),
\[
h_{2k+1,m}^{(\mu)} = \left( d_k^{(m)} \right) \gamma_{2k-2m+1}^{(\mu+m)} = \frac{2^{4k+2} \Gamma(k+\mu+\frac{3}{2})(k)!}{(k-m)!}.
\]
Then, following the same lines as above, we can show
\[
\| \Pi_N^{(\mu)} u_0 - u_0 \|_{\chi(\mu)}^2 \leq \frac{\gamma_N^{(\mu)} + 2}{h_N^{(\mu)} 2N + 2m} \| D^m u_0 \|_{\chi(\mu + m)}^2 \leq \frac{(N + 1\, m)!}{(N + 1)!} \| D^m u_0 \|_{\chi(\mu + m)}^2. \tag{3.49}
\]
Thus, a combination of (3.44), (3.47) and (3.49) leads to the estimate (3.42) with odd \( N \). For even \( N \), we can obtain the same estimate but with \( N/2 \) in place of \( (N + 1)/2 \) in the upper bound.

Now, we turn to the proof of (3.43). If \( u e^{x^2} \in B^\mu_N(\mathbb{R}) \), we find from (3.28) that
\[
\| u - \hat{\Pi}_N^{(\mu)} u \|_{\omega(\mu)} = \| u e^{x^2} - \hat{\Pi}_N^{(\mu)} (ue^{x^2}) \|_{\chi(\mu)}. \tag{3.50}
\]
Then the estimate (3.43) is a direct consequence of (3.42). \( \Box \)

4. Generalized Hermite polynomials/functions in multiple dimensions

In this section, we introduce the multi-dimensional GHPs, GHFs and their adjoint counterparts, and show that the construction renders the important properties valid in one dimension still hold.

4.1. Generalized Hermite polynomials and functions in \( \mathbb{R}^d \). For notational convenience, we introduce the index sets related to the spherical harmonics on \( S^{d-1} \) as in Subsection 2.2

\[
\begin{align*}
\Upsilon_d^\infty &= \{ (\ell, n) : 1 \leq \ell \leq a_d, \ 0 \leq n < \infty, \ \ell, n \in \mathbb{N}_0 \}, \\
\Upsilon_d^N &= \{ (\ell, n) : 1 \leq \ell \leq a_d, \ 0 \leq n \leq N, \ \ell, n \in \mathbb{N}_0 \}. \tag{4.1}
\end{align*}
\]

Definition 4.1. For \( \mu > -\frac{1}{2}, k \in \mathbb{N}_0 \) and \( (\ell, n, (\ell, n)) \in \Upsilon_d^\infty \), we define the \( d \)-dimensional generalised Hermite polynomials as
\[
H_{k, \ell}^{\mu, n}(x) := H_{k, \ell}^{\mu, n}(x; d) = L_k^{(n + \frac{d}{2} + \mu)}(|x|^2)Y_{\ell}^n(x) = r^n L_k^{(n + \frac{d}{2} + \mu)}(r^2)Y_{\ell}^n(\hat{x}), \quad x = r \hat{x}, \tag{4.2}
\]
and correspondingly, the \( d \)-dimensional generalised Hermite functions are defined as
\[
\tilde{H}_{k, \ell}^{\mu, n}(x) = \sqrt{1/\gamma_{k, n}^{\mu, d}} e^{-\frac{|x|^2}{2}} H_{k, \ell}^{\mu, n}(x), \quad \gamma_{k, n}^{\mu, d} := \frac{\Gamma(k + n + \frac{d}{2} + \mu)}{2^k k!}. \tag{4.3}
\]

The GHPs and GHFs are constructed in such a way so that they are orthogonal with respect to the weight functions as a direct extension of one-dimensional case.

Theorem 4.1. For \( \mu > -\frac{1}{2}, k, j \in \mathbb{N}_0 \) and \( (\ell, n, (\ell, n)) \in \Upsilon_d^\infty \), the GHPs are mutually orthogonal with respect to the weight function \( |x|^{2\mu} e^{-|x|^2} \), namely,
\[
\int_{\mathbb{R}^d} H_{k, \ell}^{\mu, n}(x) H_{j, \ell}^{\mu, m}(x) |x|^{2\mu} e^{-|x|^2} \, dx = \gamma_{k, n}^{\mu, d} \delta_{\mu, n} \delta_{k, j} \delta_{\ell, \ell}, \tag{4.4}
\]
and the GHFs are orthonormal
\[
\int_{\mathbb{R}^d} \tilde{H}_{k, \ell}^{\mu, n}(x) \tilde{H}_{j, \ell}^{\mu, m}(x) |x|^{2\mu} e^{-|x|^2} \, dx = \delta_{\mu, n} \delta_{k, j} \delta_{\ell, \ell}. \tag{4.5}
\]

Proof. The orthogonality (4.5) is a direct consequence of (4.3) and (4.4), so we only need to show (4.4). Using the spherical polar coordinates transformation, (3.7), (2.16) and (4.2), we obtain
\[
\begin{align*}
\int_{\mathbb{R}^d} H_{k, \ell}^{\mu, n}(x) H_{j, \ell}^{\mu, m}(x) |x|^{2\mu} e^{-|x|^2} \, dx &= \int_0^\infty L_k^{(n + \frac{d}{2} + \mu)}(r^2) L_j^{(m + \frac{d}{2} + \mu)}(r^2) r^{2\mu + 2n + d - 1} e^{-r^2} \, dx \int_{\mathbb{S}^{d-1}} Y_n^m(\hat{x}) Y_m^m(\hat{x}) \, d\sigma(\hat{x}) \\
&= \delta_{\mu, n} \delta_{\ell, \ell} \int_0^\infty L_k^{(n + \frac{d}{2} + \mu)}(r^2) L_j^{(m + \frac{d}{2} + \mu)}(r^2) r^{2\mu + 2n + d - 1} e^{-r^2} \, dr.
\end{align*}
\]
where the Burnett polynomials can be viewed as the scaled GHPs with Proposition 4.3.

\[ \frac{\Gamma(k + n + \frac{d}{2} + \mu)}{2\Gamma(k + 1)} \delta_{mn} \delta_{kj} \delta_{\ell \ell} = \gamma_{k,n}^d \delta_{mn} \delta_{kj} \delta_{\ell \ell}, \]

which yields (4.4). This ends the proof. \( \square \)

Remark 4.1. For \( d = 1, 2, 3 \), the GHFs take the forms as follows, which can be verified readily from (3.6), (4.2) and Remark 2.4.

- For \( d = 1 \), we have
  \[ H_{k,1}^{\mu,0}(x) = \frac{1}{\sqrt{2}} L_k^{(\mu-\frac{1}{2})}(x^2) = \frac{(-1)^k}{2^{2k+\frac{1}{2}} k!} H_{2k}^{(\mu)}(x), \]
  \[ H_{k,1}^{\mu,1}(x) = \frac{x}{\sqrt{2}} L_k^{(\mu+\frac{1}{2})}(x^2) = \frac{(-1)^k}{2^{2k+\frac{1}{2}} k!} H_{2k+1}^{(\mu)}(x), \] (4.6)

  where \( \{H_n^{(\mu)}\} \) are the one-dimensional GHFs as defined in Subsection 3.1.

- For \( d = 2 \), we have
  \[ H_{k,2}^{\mu,0} r^n L_k^{(\mu)}(r^2); \quad H_{k,2}^{\mu,1} r^n L_k^{(\mu+1)}(r^2) \cos(n\theta), \]
  \[ H_{k,2}^{\mu,2} r^n L_k^{(\mu+1)}(r^2) \sin(n\theta), \quad n \geq 1, \quad k \geq 0. \] (4.7)

- For \( d = 3 \), the spherical harmonic basis functions in Definition 4.1 are formed by the product of \( r^n L_k^{(n+\frac{1}{2}+\mu)}(r^2) \) and the spherical harmonics in (2.19).

Remark 4.2. It is interesting to take note of the connection between GHPs and the Burnett polynomials (which was first constructed by Burnett \[6\] and used as basis functions in solving kinetic equations (see, e.g., \[9\])). Recall that for \( d = 3 \), the Burnett polynomials are defined by

\[ B_{k,\ell}^n(x) = c_k^n r^n L_k^{(n+\frac{1}{2})}\left(\frac{r^2}{2}\right) Y_{\ell n}(x), \quad k \in \mathbb{N}_0, \quad (\ell, n) \in \mathbb{Y}^3_{\mathbb{R}}, \] (4.8)

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

\[ \int_{\mathbb{R}^3} B_{k,\ell}^n(x) B_{j m}^{n'}(x) e^{-\frac{|x|^2}{2}} \, dx = \delta_{kj} \delta_{m n} \delta_{\ell \ell}. \] (4.9)

In other words, the Burnett polynomials are mutually orthogonal with respect to the Maxwellian \( \mathcal{M}(x) = \frac{1}{(2\pi)^{d/2}} e^{-\frac{|x|^2}{2}} \). Observe from (4.2) and (4.4) (with \( d = 3 \) and \( \mu = 0 \)) that

\[ H_{k,\ell}^{0,n}(x) = c_k^n B_{k,\ell}^n(\sqrt{2} x), \] (4.10)

so the Burnett polynomials can be viewed as the scaled GHFs with \( \mu = 0 \).

Now, we present some other properties of the \( d \)-dimensional GHPs and GHFs.

Proposition 4.3. For \( \mu > -\frac{1}{2} \) and fixed \( (\ell, n) \in \mathbb{Y}^d_{\mathbb{R}}, \) we have the following recurrence relations in \( k \):

\[ (k + 1) H_{k+1,\ell}^{\mu,n}(x) = (2k + n + d/2 + \mu - |x|^2) H_{k,\ell}^{\mu,n}(x) - (k + n + d/2 - 1 + \mu) H_{k-1,\ell}^{\mu,n}(x), \] (4.11)

and for the GHFs,

\[ a_k \hat{H}_{k+1,\ell}^{\mu,n}(x) = (b_k - |x|^2) \hat{H}_{k,\ell}^{\mu,n}(x) - c_k \hat{H}_{k-1,\ell}^{\mu,n}(x), \] (4.12)

where

\[ a_k = \sqrt{(k+1)(k+n+d/2+\mu)}, \quad b_k = 2k + n + d/2 + \mu, \quad c_k = \sqrt{k(k-1+n+d/2+\mu)}. \]
According to [3, Lemma 9.10.2], we have that for any \( \hat{\mu}, \hat{\nu} > 0  \), namely,
\[
\hat{H}^{\mu, \nu}_{k, \ell}(x) = \sum_{j=0}^{k} \mu^{\nu} C_{j}^{k} \hat{H}^{\mu, \nu}_{j, \ell}(x), \quad x \in \mathbb{R}^{d}, \quad k \in \mathbb{N}_{0},
\]
where the connection coefficients are given by
\[
\mu^{\nu} C_{j}^{k} = \frac{\Gamma(k-j+\mu-\nu)}{\Gamma(\mu-\nu)(k-j)!} \sqrt{\frac{k! \Gamma(j+n+\frac{d}{2}+\nu)}{\Gamma(\beta+1)(k-j)!}}.
\]

Proof. Recall the property of the generalized Laguerre polynomials (cf. [4, (7.4)]):
\[
L_{k}^{(\mu+\beta+1)}(z) = \sum_{j=0}^{k} \frac{\Gamma(k-j+\beta+1)}{\Gamma(\beta+1)(k-j)!} L_{j}^{(\mu)}(z),
\]
which, together with (2.1) and Definition 4.1, leads to the desired result. \( \square \)

4.2. Adjoint generalized Hermite functions in \( \mathbb{R}^{d} \). In what follows, we first define the adjoint generalised Hermite functions and then show that they can preserve the properties (1.3)-(1.4) but in multiple dimensions.

Definition 4.2. For \( \mu > -\frac{1}{2}, (\ell, n) \in \mathbb{Y}_{\ell}, \) and \( k \in \mathbb{N}_{0} \), the d-dimensional adjoint GHFs are defined by
\[
\tilde{H}_{\mu, n}^{\mu, \cdot}(x) = \sum_{j=0}^{k} (-1)^{k-j} \mu^{n} C_{j}^{k} \tilde{H}_{j, \ell}^{\mu, n}(x), \quad x \in \mathbb{R}^{d},
\]
where the coefficients \( \{\mu^{n} C_{j}^{k}\} \) are given by (4.16).

As with Theorem 3.1, the d-dimensional GHFs and its adjoint enjoy the following important properties.

Theorem 4.2. For \( \mu > -\frac{1}{2}, (\ell, n) \in \mathbb{Y}_{\ell}, \) and \( k \in \mathbb{N}_{0} \), we have
\[
\mathcal{F}[\hat{H}_{k, \ell}^{\mu, n}](\xi) = (-i)^{n+2k} \hat{H}_{k, \ell}^{\mu, n}(\xi), \quad \mathcal{F}^{-1}[\tilde{H}_{k, \ell}^{\mu, n}](\xi) = i^{n+2k} \tilde{H}_{k, \ell}^{\mu, n}(\xi),
\]
and for \( s > 0 \),
\[
\mathcal{F}[(-\Delta)^s \hat{H}_{k, \ell}^{\mu, n}](\xi) = (-i)^{n+2k} |s|^{2s} \hat{H}_{k, \ell}^{\mu, n}(\xi).
\]
Moreover, the adjoint GHFs are orthonormal in the sense that
\[
((\Delta)^s \tilde{H}_{j, \ell}^{\mu, n}, (-\Delta)^s \tilde{H}_{j, \ell}^{\mu, m})_{\mathbb{R}^{d}} = \delta_{jk} \delta_{mn} \delta_{\ell\ell}.
\]
Proof. We first show that for \( \mu = 0 \), the GHFs \( \{\tilde{H}_{k, \ell}^{0, n}(x)\} \) are the eigenfunctions of the Fourier transform, namely,
\[
\mathcal{F}[\tilde{H}_{k, \ell}^{0, n}](\xi) = (-i)^{n+2k} \tilde{H}_{k, \ell}^{0, n}(\xi).
\]
According to [3] Lemma 9.10.2, we have that for any \( \tilde{x}, \tilde{\xi} \in \mathbb{S}^{d-1} \) and \( w > 0 \),
\[
\int_{\mathbb{S}^{d-1}} Y_{\ell}^{m}(\tilde{x}) e^{-i\omega \langle \tilde{\xi}, \tilde{x} \rangle} d\sigma(\tilde{x}) = \frac{(\pi)^{\frac{d}{2}}}{\omega^{\frac{d}{2}}} J_{n+\frac{d}{2}}(\omega) Y_{\ell}^{m}(\tilde{\xi}),
\]
where \( J_\nu(z) \) is the Bessel functions of the first kind of order \( \nu \) as in [1]. Then using Definition 4.1 with \( \mu = 0 \), and (4.23) with \( \omega = \rho r \) and \( \rho = |\xi| \), leads to

\[
\hat{F}[\hat{H}_{k,\ell}^{0,n}(\xi)] = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \hat{H}_{k,\ell}^{0,n}(x)e^{-i\langle \xi, x \rangle} \, dx
\]

\[
= \frac{1}{\sqrt{|\gamma|_{k,n}}} \int_0^\infty \int_{S^{d-1}} r^n L_k^{(n+d-2)}(r^2) e^{-\frac{r^2}{2}} \left\{ \int_{S^{d-1}} Y_\ell^n(\hat{\sigma}) e^{-i\rho r \langle \hat{\sigma}, \hat{\xi} \rangle} \, d\sigma(\hat{\sigma}) \right\} r^{d-1} \, dr
\]

(4.24)

Recall the integral identity of the generalised Laguerre polynomials (cf. [23, P. 820]): for \( \alpha > -1 \) and \( k \in \mathbb{N}_0 \),

\[
\int_0^\infty r^{\alpha+1} L_k^{(\alpha)}(r^2) e^{-\frac{r^2}{2}} J_\alpha(\rho r) \, dr = (-1)^k \rho^\alpha L_k^{(\alpha)}(\rho^2) e^{-\frac{\rho^2}{2}}, \quad \rho > 0.
\]

(4.25)

Thus, taking \( \alpha = n + \frac{d-2}{2} \) in (4.25), we can evaluate the integral in (4.24) and derive from (4.3) with \( \mu = 0 \) that

\[
\hat{F}[\hat{H}_{k,\ell}^{0,n}(\xi)] = \frac{(-1)^k}{\sqrt{|\gamma|_{k,n}}} \int_0^\infty r^{n+\frac{d-2}{2}} L_k^{(n+d-2)}(r^2) e^{-\frac{r^2}{2}} Y_\ell^n(\hat{\xi}) = (-1)^{n+2k} \hat{H}_{k,\ell}^{0,n}(\xi).
\]

This yields (4.22).

From Definition 4.2 and the property (4.22), we obtain

\[
\hat{F}[\hat{H}_{k,\ell}^{\mu,n}(\xi)] = \sum_{j=0}^k (-1)^{k-j} \frac{\mu C_j}{0 C_j} \hat{F}[\hat{H}_{j,\ell}^{0,n}(\xi)] = \sum_{j=0}^k (-1)^{k-j} \frac{\mu C_j}{0 C_j} \hat{H}_{j,\ell}^{0,n}(\xi)
\]

(4.26)

\[
= (-1)^{n+2k} \sum_{j=0}^k \frac{\mu C_j}{0 C_j} \hat{H}_{j,\ell}^{0,n}(\xi) = (-1)^{n+2k} \hat{H}_{k,\ell}^{n,n}(\xi),
\]

where in the last step, we used (4.15). This gives the first identity of (4.19), which yields the second identity immediately.

The property (4.20) is a direct consequence of (4.19) and the definition of fractional Laplacian by Fourier transform.

Finally, using the Parseval’s identity and (4.20), we derive from the orthogonality (4.5) that

\[
((-\Delta)^{s} \hat{H}_{k,\ell}^{s,n}, (-\Delta)^{s} \hat{H}_{j,\ell}^{s,m})_{\mathbb{R}^d} = \langle \hat{F}[(-\Delta)^{s} \hat{H}_{k,\ell}^{s,n}], \hat{F}[(-\Delta)^{s} \hat{H}_{j,\ell}^{s,m}] \rangle_{\mathbb{R}^d}
\]

\[
= (-1)^{n+m+2k-2j} \langle \xi \rangle^{2s} \hat{H}_{k,\ell}^{s,n}, \hat{H}_{j,\ell}^{s,m} \rangle_{\mathbb{R}^d} = \delta_{mn} \delta_{kj} \delta_{\ell \ell}.
\]

This yields (4.21) and ends the proof.

\( \square \)

**Remark 4.3.** It is worthwhile to point out that the A-GHFs with \( s = 1 \)

\[
\hat{H}_{k,\ell}^{1,n}(x) = \sqrt{\frac{k!}{\Gamma(k+n+\frac{d}{2}+1)}} \sum_{j=0}^{k} \frac{\Gamma(j+n+\frac{d}{2})}{j!} \hat{H}_{j,\ell}^{0,n}(x),
\]

are Sobolev orthogonal with respect to usual Laplacian operator, i.e.,

\[
\langle \nabla \hat{H}_{k,\ell}^{1,n}, \nabla \hat{H}_{j,\ell}^{1,m} \rangle_{\mathbb{R}^d} = \delta_{kj} \delta_{mn} \delta_{\ell \ell}.
\]

However, this attractive property does not hold for the usual Hermite spectral methods based on tensorial Hermite functions \( \prod_{j=1}^{d} \hat{H}_{j}(x_j) \). Thus, it is advantageous to choose such a basis for usual Laplacian and bi-harmonic Laplacian (using the A-GHFs with \( s = 2 \)) in \( \mathbb{R}^d \).
Remark 4.4. We also point out that the eigen-functions of the finite Fourier transform are the ball prolate spheroidal wave functions defined in [33], which provide a useful tool for approximating bandlimited functions.

5. Applications: GHF-spectral-Galerkin methods for fractional Laplacian

As an immediate consequence of the attractive property (4.21), the use of A-GHFs as basis functions can lead to identity stiffness matrix for the integral fractional Laplacian. We elaborate details and conduct the error analysis in this section.

5.1. GHF-spectral-Galerkin scheme. As an illustrative example, we consider

\begin{align}
\begin{cases}
(-\Delta)^s u(x) + \gamma u(x) = f(x) & \text{in } \mathbb{R}^d, \\
u(x) = 0 & \text{as } |x| \to \infty,
\end{cases}
\tag{5.1}
\end{align}

where \( s \in (0, 1), \gamma > 0, f \in H^{-s}(\mathbb{R}^d) \), and the fractional Laplacian operator is defined in (2.2)-(2.3).

A weak formulation of (5.1) is to find \( u \in H^s(\mathbb{R}^d) \) such that

\begin{align}
A_s(u, v) &= ((-\Delta)^s u, (-\Delta)^s v)_{\mathbb{R}^d} + \gamma (u, v)_{\mathbb{R}^d}, \quad \forall v \in H^s(\mathbb{R}^d).
\tag{5.2}
\end{align}

By the definitions (2.2) and (2.4), we immediately obtain the continuity and coercivity of the bilinear form \( A_s(\cdot, \cdot) \), that is, for any \( u, v \in H^s(\mathbb{R}^d) \),

\begin{align}
|A_s(u, v)| &\lesssim \|u\|_{H^s(\mathbb{R}^d)} \|v\|_{H^s(\mathbb{R}^d)}, \\
|A_s(u, u)| &\gtrsim \|u\|_{H^s(\mathbb{R}^d)}^2.
\tag{5.3}
\end{align}

Here, the notation \( A \lesssim B \) means there exists a positive constant \( c \), independent of any function and discretization parameters, such that \( A \leq cB \). Then according to the Lax-Milgram lemma (cf. 3), the problem (5.2) admits a unique solution satisfying \( \|u\|_{H^s(\mathbb{R}^d)} \lesssim \|f\|_{H^{-s}(\mathbb{R}^d)} \).

We choose the finite dimensional approximation space spanned by the \( d \)-dimensional GHFs in Definition 1.1 or equivalently by the A-GHFs in Definition 1.2. However, in view of (4.21), it is advantageous to use the latter as the basis functions, so we define

\begin{align}
\mathcal{V}_N^d := \text{span}\{ \tilde{H}_{k,\ell}^{n,n}(x) : 0 \leq n \leq N, 1 \leq \ell \leq a_n^d, 0 \leq 2k \leq N - n, k, \ell, n \in \mathbb{N}_0 \}.
\tag{5.4}
\end{align}

Then, the spectral-Galerkin approximation to (5.2) is to find \( u_N \in \mathcal{V}_N^d \) such that

\begin{align}
A_s(u_N, v_N) = (f, v_N)_{\mathbb{R}^d}, \quad \forall v_N \in \mathcal{V}_N^d.
\tag{5.5}
\end{align}

As with the continuous problem (5.2), it admits a unique solution in \( \mathcal{V}_N^d \).

We now derive the corresponding linear system. We first write

\begin{align}
u_N(x) = \sum_{n=0}^{N} a_n^d \sum_{\ell=1}^{\frac{2n}{a_n^d}} \tilde{u}_{k,\ell}^{n,n}(x),
\tag{5.6}
\end{align}

and arrange the unknown coefficients in the order

\begin{align}
u = (\tilde{u}_0^0, \tilde{u}_0^1, \tilde{u}_1^0, \tilde{u}_1^1, \cdots, \tilde{u}_{a_n^d-1}^0, \tilde{u}_{a_n^d}^1, \cdots, \tilde{u}_{a_n^d-1}^1, \cdots, \tilde{u}_{a_n^d}^N, \cdots, \tilde{u}_{a_n^d}^N)^t,
\tag{5.7}
\end{align}

\begin{align}\tilde{u}_n^0 = (\tilde{u}_0^0, \tilde{u}_1^0, \cdots, \tilde{u}_{a_n^d-1}^0, \tilde{u}_{a_n^d}^1, \cdots, \tilde{u}_{a_n^d}^n, \cdots, \tilde{u}_{a_n^d}^N)^t,
\tag{5.8}
\end{align}

and likewise for \( f \), but with the components \( \tilde{f}_{k,\ell}^{n,n} = (f, \tilde{H}_{k,\ell}^{n,n})_{\mathbb{R}^d} \).

The orthogonality (4.21) implies that the stiffness matrix is an identity matrix. Moreover, in view of the orthogonality of the spherical harmonic basis (cf. (2.16)), the corresponding mass matrices are block diagonal.

\begin{align}
M = \text{diag}\{ M_0^0, M_1^0, \cdots, M_{a_n^d}^0, M_0^1, M_1^1, \cdots, M_{a_n^d}^1, \cdots, M_0^N, M_1^N, \cdots, M_{a_n^d}^N \}.
\tag{5.9}
\end{align}
where the entries of each diagonal block \((M^p_\alpha)_{kj}\) can be computed by
\[
(M^p_\alpha)_{kj} = \langle \tilde{H}^{\alpha,n}_{k,j}, \tilde{H}^{\alpha,n}_{j,k} \rangle_{\mathbb{R}^d} = \sum_{p=0}^{k} (-1)^{k-p} s_p^k \sum_{q=0}^{j} (-1)^{j-q} s_q^j \langle \tilde{H}^{\alpha,n}_{p,k}, \tilde{H}^{\alpha,n}_{q,l} \rangle_{\mathbb{R}^d}
\]
(5.9)
Thus the linear system of (5.5) can be written as
\[
(I + \gamma M)u = f.
\]
(5.10)

With the new basis at our proposal, the above method has remarkable advantages over the existing Hermite approaches (cf. [31, 51]). Although the usual one-dimensional Hermite functions are eigenfunctions of Fourier transform, we observe from the definition (2.2) that the factor \(|\xi|^{2\alpha}\) is non-separable, so the use of tensorial Hermite functions leads to a dense stiffness matrix whose entries are difficult to evaluate due to the involved singularity.

5.2. Error analysis. Applying the first Strang lemma [47] for the standard Galerkin framework (i.e., (5.2) and (5.5)), we obtain immediately that
\[
\|u - u_N\|_{H^s(\mathbb{R}^d)} \leq \inf_{v_N \in V_N^d} \|u - v_N\|_{H^s(\mathbb{R}^d)}.
\]
(5.11)
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 \(\pi_N^d : L^2(\mathbb{R}^d) \rightarrow V_N^d\) such that
\[
(\pi_N^d u, v)_{\mathbb{R}^d} = 0, \quad \forall v \in V_N^d.
\]
(5.12)
From Definition 4.2 and with a change of basis functions, we find readily that
\[
V_N^d := \text{span}\{\tilde{H}^{\alpha,n}_{k,j}(x) : 0 \leq n \leq N, 1 \leq \ell \leq a^d_\alpha, 0 \leq 2k \leq N - n, k, \ell, n \in \mathbb{N}_0\}.
\]
(5.13)
Thus, we can equivalently write
\[
\pi_N^d u(x) = \sum_{n=0}^{N} \sum_{\ell=1}^{a^d_\alpha} \sum_{k=0}^{\lfloor N/2 \rfloor} \tilde{u}^{\alpha,n}_{k,\ell} \tilde{H}^{\alpha,n}_{k,\ell}(x).
\]
(5.14)
We first make necessary preparations, and present the following important property.

Lemma 5.1. For \(k \in \mathbb{N}_0, (\ell, n) \in \mathcal{Y}^d_{\alpha}\), the GHFs with \(\mu = 0\) satisfy
\[
\left(-\Delta + |x|^2\right) \tilde{H}^{\alpha,n}_{k,j}(x) = (4k + 2n + d) \tilde{H}^{\alpha,n}_{k,j}(x).
\]
(5.15)
Proof. Recall the Lemma 2.1 in [32] with \(\alpha = n + d/2 - 1\) and \(\beta = \alpha + 1 - d/2\),
\[
\left[\partial_r^2 + \frac{d-1}{r} \partial_r - \frac{n(n + d - 2)}{r^2}\right] - r^2 + 4k + 2n + d\left[r^n L_k^{(n+d/2-1)}(r^2) e^{-r^2/2}\right] = 0.
\]
(5.16)
Thanks to \(Y(x) = r^n Y(t)\), (2.14), (2.17), (4.2), (4.3) and (5.16), we conclude that
\[
-\Delta \tilde{H}^{\alpha,n}_{k,j}(x) = -\sqrt{1/\gamma_{k,n}} \left[\partial_r^2 + \frac{d-1}{r} \partial_r - \frac{n(n + d - 2)}{r^2}\right] - r^2 + 4k + 2n + d\left[r^n L_k^{(n+d/2-1)}(r^2) e^{-r^2/2}\right] Y(\hat{x})
\]
\[
= \sqrt{1/\gamma_{k,n}} \left[-r^2 + 4k + 2n + d\right] \left[r^n L_k^{(n+d/2-1)}(r^2) e^{-r^2/2}\right] Y(\hat{x})
\]
\[
= (r^2 + 4k + 2n + d) \tilde{H}^{\alpha,n}_{k,j}(x),
\]
which gives the desired result (5.15).
Based on (5.15), we introduce the function space $\mathcal{B}^r(\mathbb{R}^d)$ equipped with the norm
\[
\|u\|_{\mathcal{B}^r(\mathbb{R}^d)}^2 = \begin{cases} 
\|(-\Delta + |x|^2)^m u\|_{L^2(\mathbb{R}^d)}^2, & r = 2m, \\
\frac{1}{2} \left( \| (x + \nabla)(-\Delta + |x|^2)^m u\|_{L^2(\mathbb{R}^d)}^2 + \| (x - \nabla)(-\Delta + |x|^2)^m u\|_{L^2(\mathbb{R}^d)}^2 \right), & r = 2m + 1,
\end{cases}
\] (5.18)
where integer $r \geq 0$.

The main approximation result is stated below.

**Theorem 5.1.** Let $s \in (0, 1)$. For any $u \in \mathcal{B}^r(\mathbb{R}^d)$ with integer $r \geq 1$, we have
\[
\|\pi_N^d u - u\|_{L^2(\mathbb{R}^d)} \leq (2N + d + 2)^{(s-r)/2}\|u\|_{\mathcal{B}^r(\mathbb{R}^d)}. 
\] (5.19)

**Proof.** (i). We first estimate the $L^2$-error. For $r = 2m + 1$, a direct calculation gives
\[
\|u\|_{\mathcal{B}^r(\mathbb{R}^d)}^2 = \frac{1}{2} \left( \| (x + \nabla)(-\Delta + |x|^2)^m u\|_{L^2(\mathbb{R}^d)}^2 + \| (x - \nabla)(-\Delta + |x|^2)^m u\|_{L^2(\mathbb{R}^d)}^2 \right) 
= \left( (-\Delta + |x|^2)^m + u, (-\Delta + |x|^2)^m u\right)_{\mathbb{R}^d},
\] (5.20)

Thanks to the orthogonality (4.15), (5.15)-(5.18) and (5.20), we have that for any $r \geq 0$,
\[
\|u\|_{\mathcal{B}^r(\mathbb{R}^d)}^2 = \sum_{n=0}^{\infty} \sum_{\ell=1}^{d} h_{k,d}^{n,\ell} |\tilde{u}_{k,\ell}|^2, 
\] (5.21)

Then, we derive from (5.14) and (5.21) that
\[
\|\pi_N^d u - u\|_{L^2(\mathbb{R}^d)}^2 = \sum_{n=0}^{\infty} \sum_{\ell=1}^{d} \sum_{k=\frac{N+1-n}{2}}^{N} h_{k,d}^{n,\ell} |\tilde{u}_{k,\ell}|^2 
\leq \max_{2k+n>N+1} \left\{ h_{k,d}^{n,\ell} \right\} \sum_{n=0}^{\infty} \sum_{\ell=1}^{d} \sum_{k=\frac{N+1-n}{2}}^{N} h_{k,d}^{n,\ell} |\tilde{u}_{k,\ell}|^2 
\leq (2N + d) \|u\|_{\mathcal{B}^r(\mathbb{R}^d)},
\] (5.22)

If $r = 2m$, we find from (5.18) that (5.20) simply becomes
\[
\|u\|_{\mathcal{B}^r(\mathbb{R}^d)}^2 = \left( (-\Delta + |x|^2)^m u, (-\Delta + |x|^2)^m u\right)_{\mathbb{R}^d},
\] (5.23)
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 (5.20), we obtain that
\[
\|\nabla(\pi_N^d u - u)\|_{L^2(\mathbb{R}^d)}^2 \leq \frac{1}{2} \left( \| (x + \nabla)(\pi_N^d u - u)\|_{L^2(\mathbb{R}^d)}^2 + \| (x - \nabla)(\pi_N^d u - u)\|_{L^2(\mathbb{R}^d)}^2 \right) 
= \left( (-\Delta + |x|^2)(\pi_N^d u - u), (\pi_N^d u - u)\right)_{\mathbb{R}^d} \leq \sum_{n=0}^{\infty} \sum_{\ell=1}^{d} \sum_{k=\frac{N+1-n}{2}}^{N} h_{k,d}^{n,\ell} |\tilde{u}_{k,\ell}|^2 
\leq \max_{2k+n>N+1} \left\{ h_{k,d}^{n,\ell} \right\} \sum_{n=0}^{\infty} \sum_{\ell=1}^{d} \sum_{k=\frac{N+1-n}{2}}^{N} h_{k,d}^{n,\ell} |\tilde{u}_{k,\ell}|^2 
\leq (2N + d)^{1-r}\|u\|_{\mathcal{B}^r(\mathbb{R}^d)}. 
\] (5.24)

Finally, the desired results can be obtained by the space interpolation inequality (2.8) and the $L^2$- and $H^1$-bounds derived above. $\Box$

Taking $v_N = \pi_N^d u$ in (5.11) and using Theorem 5.1, we immediately obtain the following error estimate.
Theorem 5.2. Let \( u \) and \( u_N \) be the solutions to (5.2) and (5.5), respectively. If \( u \in \mathcal{B}^r(\mathbb{R}^d) \) with integer \( r \geq 1 \), then we have
\[
\|u - u_N\|_{\mathcal{B}^s(\mathbb{R}^d)} \lesssim (2N + d + 2)^{(s-r)/2}\|u\|_{\mathcal{B}^r(\mathbb{R}^d)}, \quad s \in (0, 1).
\] (5.25)

5.3. 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 (5.6), so the numerical solution takes the form
\[
u_{N,K}(x) = \sum_{n=0}^{N} \sum_{\ell=1}^{K} \tilde{u}_{n}^{\ell} \tilde{H}_{n}^{\mu,n}(x), \quad d \geq 2,
\] (5.26)
and
\[
u_{N}(x) = \sum_{n=0}^{N} \tilde{u}_{n} \tilde{H}_{n}^{(\mu)}(x), \quad d = 1.
\] (5.27)

Example 1. (Problem (5.1) with exact solution). We first consider (5.1) with the following exact solutions:
\[
u_{e}(x) = e^{-|x|^2}, \quad \nu_{a}(x) = (1 + |x|^2)^{-r}, \quad r > 0, \quad x \in \mathbb{R}^d.
\] (5.28)

According to [45] Proposition 4.2 & 4.3, the source terms \( f_e(x) \) and \( f_a(x) \) are respectively given by
\[
f_e(x) = \gamma e^{-|x|^2} + \frac{2^{2s} \Gamma(s + d/2)}{\Gamma(d/2)} F_1\left(s + \frac{d}{2}; \frac{d}{2}; -|x|^2\right),
\]
\[
f_a(x) = \gamma (1 + |x|^2)^{-r} + \frac{2^{2s} \Gamma(s + r) \Gamma(s + d/2)}{\Gamma(r) \Gamma(d/2)} F_2\left(s + r, s + \frac{d}{2}; -|x|^2\right).
\]

For \( d = 1 \), we plot the maximum errors, in semi-log scale and log-log scale, in Figure 5.1 (a)-(b) for \( u_e \) and \( u_a \), respectively. Here we take \( s = 0.3, 0.5, 0.7 \) and various \( N \). For \( d = 2, 3 \), we take \( s = 0.3, 0.5, 0.7 \) and the degree in angular direction is fixed \( N = 10 \) (see (5.26)). In Figure 5.1 (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 algebraical convergence for \( u_e \) and \( u_a \), respectively.

Example 2. (Problem (5.1) with a source term). We next consider (5.1) with the following source functions:
\[
f_e(x) = \sin(|x|)e^{-|x|^2}, \quad f_a(x) = \cos(|x|)(1 + |x|^2)^{-r}, \quad r > 0, \quad x \in \mathbb{R}^d.
\] (5.29)

The exact solutions are unknown, and we use the numerical solution with \( K = 80, N = 20 \) as the reference solution. In Figure 5.2 (a)-(b), we plot in log-log scale the maximum errors of (5.1) against various \( N \) with \( s = 0.3, 0.5, 0.7 \) for \( d = 1 \). For \( d = 2, 3 \), we plot the maximum errors, in log-log scale, for (5.1) against various \( K \) in Figure 5.2 (c)-(f), which we take \( s = 0.3, 0.5, 0.7 \) and fix \( N = 10 \). As shown in [45], the solution of (5.1) decays algebraically, even for exponentially decaying source terms. Indeed, we observe an algebraic order of convergence.

6. Applications: eigenvalue problems involving Schrödinger operators

In this section, we consider the Hermite spectral approximation to the eigenvalue problem with the Schrödinger operator:
\[
\begin{cases}
\left[-\frac{1}{2}\Delta + V(x)\right] u(x) = \lambda u(x) \quad \text{in} \quad \mathbb{R}^d, \\
u(x) = 0 \quad \text{as} \quad |x| \to \infty,
\end{cases}
\] (6.1)

where the potential function \( V(x) = Z|x|^\alpha \) with \( \alpha, Z \) being given constants. It is known that (i) if \( \alpha > -1 \), all eigenvalues of (6.1) are distinct; (ii) if \( \alpha = -1 \) or \( Z = 0 \), the spectrum of the Schrödinger
The maximum errors of the GHF-spectral-Galerkin scheme with $\gamma = 1$ for Example 1 with exact solutions in (5.28). Here $s = 0.3$, 0.5, 0.7.

The variational form of (6.1) is to find $\lambda \in \mathbb{R}$ and $u \in H^1(\mathbb{R}^d) \setminus \{0\}$ such that

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

In general, the fractional power potential $|x|^{2\alpha}$ induces strong singularities at the origin and results in different decaying behaviours of the eigenfunctions at infinity. The naive use of the Hermite spectral method based on the GHFs defined in (4.3) may fail to capture the singularity, so can only offer a
very limited order of convergence, after all they are polynomials in radial direction. In order to fit the singularities and obtain an exponential order of convergence, we introduce the Müntz-type GHFs and develop efficient spectral method for (6.2). As we shall see below, the new GHFs are not algebraic polynomials (in radial direction) in most cases, but Müntz polynomials. The interested readers are referred to [36, 48, 44, 29] for more details of the Müntz polynomials and their applications in spectral methods in one dimension.

6.1. Müntz-type generalised Hermite functions. To solve (6.2) accurately and efficiently, we introduce the following Müntz-type GHFs that are orthogonal in the sense of (6.5) below.
Definition 6.1. For \( \theta > 0, (\ell, n) \in \mathbb{Y}_d^d \), and \( k \in \mathbb{N}_0 \), the M"untz-type GHFs are defined by
\[
\hat{H}^{\theta,n}_{k,\ell}(x) = 
\begin{cases}
\theta_d^d L^{(\beta_n)}(x) |x|^{2\theta} e^{-\frac{|x|^2}{\theta}} Y_{\ell}^n(x), & x \in \mathbb{R}^d,
\end{cases}
\quad (6.3)
\]
where
\[
\theta_d^d = \sqrt{\frac{2k!}{\Gamma(k + \beta_n + 1)}}, \quad \beta_n = \frac{n + d/2 - 1}{\theta}.
\]

It is seen from (4.3) and (6.3) that if \( \theta = 1 \), it reduces the GHFs \( \hat{H}^{0,n}_{k,\ell}(x) \), i.e., \( \hat{H}^{1,n}_{k,\ell}(x) = \hat{H}^{0,n}_{k,\ell}(x) \).

Theorem 6.1. For \( \theta > \max(1 - d/2, 0) \), \((\ell, n), (i, m) \in \mathbb{Y}_d^d \), and \( k, j \in \mathbb{N}_0 \), we have
\[
[ - \Delta + \theta^2 |x|^{4\theta - 2} ] \hat{H}^{\theta,n}_{k,\ell}(x) = 2\theta^2 (\beta_n + 2k + 1) |x|^{2\theta - 2} \hat{H}^{\theta,n}_{k,\ell}(x),
\]
and the orthogonality
\[
(\nabla \hat{H}^{\theta,n}_{k,\ell}, \nabla \hat{H}^{\theta,m}_{j,\ell})_{\mathbb{R}^d} + 2\theta^2 (|x|^{4\theta - 2}\hat{H}^{\theta,n}_{k,\ell}, \hat{H}^{\theta,m}_{j,\ell})_{\mathbb{R}^d} \theta^2 (\beta_n + 2k + 1) \delta_{kj} \delta_{mn} \delta_{\ell\ell}.
\]

Proof. We can derive from (2.14), (2.17), (5.15), (6.3) and the change of variable \( \rho = r^\theta \) that
\[
\begin{aligned}
[ - \Delta + \theta^2 r^{4\theta - 2} ] \hat{H}^{\theta,n}_{k,\ell}(x)
&= \theta_d^d L^{(\beta_n)}(x) |x|^{2\theta} e^{-\frac{|x|^2}{\theta}} Y_{\ell}^n(x)
\end{aligned}
\]
and the orthogonality
\[
(\nabla \hat{H}^{\theta,n}_{k,\ell}, \nabla \hat{H}^{\theta,m}_{j,\ell})_{\mathbb{R}^d} + 2\theta^2 (|x|^{4\theta - 2} \hat{H}^{\theta,n}_{k,\ell}, \hat{H}^{\theta,m}_{j,\ell})_{\mathbb{R}^d} \theta^2 (\beta_n + 2k + 1) \delta_{kj} \delta_{mn} \delta_{\ell\ell}.
\]

Next, we prove the orthogonality (6.5). By virtue of (6.4), we have from (6.3) and the change of variable \( \rho = r^\theta \) that
\[
\begin{aligned}
(\nabla \hat{H}^{\theta,n}_{k,\ell}, \nabla \hat{H}^{\theta,m}_{j,\ell})_{\mathbb{R}^d} + 2\theta^2 (|x|^{4\theta - 2} \hat{H}^{\theta,n}_{k,\ell}, \hat{H}^{\theta,m}_{j,\ell})_{\mathbb{R}^d}
&= 2\theta^2 (\beta_n + 2k + 1) \theta_d^d L^{(\beta_n)}(\rho) L^{(\beta_n)}(\rho) e^{-\frac{\rho^2}{\theta}} Y_{\ell}^n(x)
\end{aligned}
\]
This completes the proof.

As a special case of (6.4) (i.e., \( \theta = \frac{1}{2} \)), we can find the explicit representation of the eigen-pairs of the Schrödinger operator with Coulomb potential: 
\[ -\frac{1}{2} \Delta - \frac{|Z|}{|x|} \] in \( d \) dimension, where \( Z \) is a nonzero constant.
Corollary 6.1. For any \( k \in \mathbb{N}_0 \), \((\ell, n) \in \Upsilon^d_{\infty}\) and \( Z \neq 0 \), we have

\[
\left[-\frac{1}{2} \Delta - \frac{|Z|}{|x|} \right]_{k,\ell}^{i,\ell,n} \left( \frac{4|Z|x}{2n+2k+d-1} \right) = -\frac{2Z^2}{(2n+2k+d-1)^2} \hat{H}_{k,\ell}^{\frac{n}{2}} \left( \frac{4|Z|x}{2n+2k+d-1} \right).
\]  

(6.6)

Proof. Taking \( \theta = \frac{1}{2} \) in \((6.4)\) and rearranging the terms, leads to

\[
\left[-\Delta - \frac{\beta_n + 2k + 1}{2|x|} \right]_{k,\ell}^{i,\ell,n} (x) = -\frac{1}{4} \hat{H}_{k,\ell}^{\frac{n}{2}} (x).
\]

With a rescaling: \( x \rightarrow \frac{4|Z|x}{\beta_n + 2k + 1} = \frac{4|Z|x}{2n+2k+d-1} \) (in \( r \) direction), we can obtain \((6.6)\) immediately. \( \square \)

The identity in Corollary 6.1 implies that the spectra of the Schrödinger operator with Coulomb potential are given by

\[
\{ \lambda_i, u_{i,\ell} \} := \left\{ \frac{2Z^2}{(2i+d-3)^2}, \hat{H}_{i-n-1,\ell}^{\frac{n}{2}} \left( \frac{4|Z|x}{2i+d-3} \right) \right\}, \quad (\ell, n) \in \Upsilon^d_{i-1}, \, i \in \mathbb{N},
\]

and the multiplicity of each \( \lambda_i \) is

\[
m_i := a_0^d + a_1^d + \cdots + a_{d-1}^d = \frac{(i-1)(d-1) + (i)(d-1)}{(d-1)!}, \quad d \geq 2,
\]

where we recall that \( a_i^d \) (defined in \((2.11)\)) is the cardinality of \( \Upsilon^d_i \setminus \Upsilon^d_{i-1} \) (defined in \((4.1)\)).

Remark 6.1. 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., [39] P. 132 and [22] Thm. 10.10 for \( d = 3 \) with a different derivation, and the recent work [38] for the asymptotic study of the eigenfunctions.

Although the orthogonality \((6.5)\) does not imply the orthogonality of each individual term, the stiffness and (weighted) mass matrices are sparse with finite bandwidth.

Theorem 6.2. For \( \theta > \max(1-d/2, 0) \), \((\ell, n), (\iota, m) \in \Upsilon^d_{\infty}\) and \( k, j \in \mathbb{N}_0 \), we have

\[
(\nabla \hat{H}_{k,\ell}^{\theta,n}, \nabla \hat{H}_{j,\iota}^{\theta,m})_{\mathbb{R}^d} = \delta_{mn} \delta_{\ell \iota} \times \begin{cases} \theta (\beta_n + 2k + 1), & j = k, \\ \theta (k + 1)(\beta_n + k + 1), & j = k + 1, \\ \theta (j + 1)(\beta_n + j + 1), & k = j + 1, \\ 0, & \text{otherwise}, \end{cases}
\]

(6.8)

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

\[
(|x|)^{2\alpha} (\hat{H}_{k,\ell}^{\theta,n}, \hat{H}_{j,\iota}^{\theta,m})_{\mathbb{R}^d} = \frac{1}{2^d} \hat{H}_{k,\ell}^{\theta,n} \hat{H}_{j,\iota}^{\theta,m} \delta_{mn} \delta_{\ell \iota} 
\]

\[
\times \sum_{p=0}^{\min(k,j)} \frac{\Gamma(k+p+1-\frac{1+\alpha}{\theta}) \Gamma(j+p+1-\frac{1+\alpha}{\theta}) \Gamma(p+\beta_n+1+\alpha)}{\Gamma^2(1-\frac{1+\alpha}{\theta})(k-p)!(j-p)!p!}
\]

(6.9)
Proof. In view of the definition (6.3), we derive from (2.16), (3.7), (4.17) and the change of variable \( \rho = r^{2\theta} \), we derive

\[
\left( |x|^{2\alpha} \mathcal{H}_{k,\ell}^{\theta,n} \right)_{\mathbb{R}^d} = c_{k,n}^{\theta,d} \int_0^\infty \rho^{n+d-1+2\alpha} L_k^{(\beta_n)}(\rho) \rho \, e^{-\rho} \, d\rho
\]

where \( \rho = \frac{x}{\|x\|} \), and \( \beta_n = \frac{\ell(\ell + d - 1) + n}{2} \). Note that (6.11) can be also obtained from (6.10) that

\[
\left( |x|^{4\theta - 2} \mathcal{H}_{k,\ell}^{\theta,n} \right)_{\mathbb{R}^d} = \frac{c_{k,n}^{\theta,d}}{2\theta} \delta_{mn} \delta_{\ell \ell} \sum_{p=0}^{\min(k,j)} \Gamma(k-p+\frac{\theta-1}{\theta}) \Gamma(j+\frac{\theta-1}{\theta}) \Gamma(p+\frac{n+d+2}{\theta})(\frac{\Gamma(j+\frac{\theta-1}{\theta})}{\Gamma(k-p+\frac{\theta-1}{\theta})})(j-p)! p!
\]

which gives (6.9). In particular, if \( \alpha = 2\theta - 1 \), we derive from (6.10) that

\[
\left( |x|^{4\theta - 2} \mathcal{H}_{k,\ell}^{\theta,n} \right)_{\mathbb{R}^d} = \frac{c_{k,n}^{\theta,d}}{2\theta} \delta_{mn} \delta_{\ell \ell} \sum_{p=0}^{\min(k,j)} \Gamma(k-p+\frac{\theta-1}{\theta}) \Gamma(j+\frac{\theta-1}{\theta}) \Gamma(p+\frac{n+d+2}{\theta})(\frac{\Gamma(j+\frac{\theta-1}{\theta})}{\Gamma(k-p+\frac{\theta-1}{\theta})})(j-p)! p!
\]

Then (6.8) is a direct consequence of (6.5) and (6.11). Note that (6.11) can be also obtained from (6.10) with the understanding \( \Gamma(z) = 1 \) if \( z \) is negative integer. \( \square \)

6.2. Numerical schemes and results.

6.2.1. Schrödinger eigenvalue problem with a Coulomb potential. In what follows, we implement the Hermite spectral method for the three-dimensional Schrödinger eigenvalue problem (6.1) with a Coulomb potential \( V(x) = \frac{Z}{\|x\|} \) with \( Z < 0 \) for the hydrogen atom [40], that is,

\[
\frac{1}{2} \Delta u(x) + \frac{Z}{\|x\|} u(x) = \lambda u(x), \quad x \in \mathbb{R}^3.
\]

Numerical solution of (6.12) 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 GHPs with a suitable parameter \( \theta = \frac{1}{2} \), in light of the Coulomb potential.

Define the approximation space

\[
\mathcal{W}_{N,K} = \text{span}\{\mathcal{H}_{k,\ell}^{\frac{1}{2}}(\kappa|x|) : 0 \leq n \leq N, 1 \leq \ell \leq 2n + 1, 0 \leq k \leq K, k, \ell, n \in \mathbb{N}_0\},
\]

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., [50, 43]). The spectral approximation scheme for (6.2) is to find \( \lambda_{N,K} \in \mathbb{R} \) and \( u_{N,K} \in \mathcal{W}_{N,K} \setminus \{0\} \) such that

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

In real implementation, we write

\[
u_{N,K}(x) = \sum_{n=0}^{N} \sum_{\ell=1}^{2n+1} \sum_{k=0}^{K} \hat{u}_{k,\ell}^{\frac{n}{2}} \mathcal{H}_{k,\ell}^{\frac{1}{2}}(\kappa|x|),
\]
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and denote
\[ \hat{u}_k^n = (\hat{u}_0^0, \hat{u}_1^0, \ldots, \hat{u}_{K-1}^0)^t, \quad u = (\hat{u}_1^1, \hat{u}_2^1, \ldots, \hat{u}_N^N, \hat{u}_2^N, \ldots, \hat{u}_{2N+1}^N)^t. \] (6.14)

With this ordering, we denote the stiffness and the mass matrices by \( S \) and \( M \), respectively, with the entries given by
\[
\mathcal{B}(\hat{H}_{k,\ell}^4(n), \hat{H}_{j,\ell}^4(m)(\kappa)) = \frac{1}{2\kappa}[(\nabla \hat{H}_{k,\ell}^4(n), \nabla \hat{H}_{j,\ell}^4(m))_{\mathbb{R}^3} + \frac{1}{4}(\hat{H}_{k,\ell}^4(n), \hat{H}_{j,\ell}^4(m))_{\mathbb{R}^3}]
+ \frac{Z}{\kappa^2}(|x|^{-1} \hat{H}_{k,\ell}^4(n), \hat{H}_{j,\ell}^4(m))_{\mathbb{R}^3} - \frac{1}{8\kappa}(\hat{H}_{k,\ell}^4(n), \hat{H}_{j,\ell}^4(m))_{\mathbb{R}^3},
\]
\[
(\hat{H}_{k,\ell}^4(n), \hat{H}_{j,\ell}^4(m)(\kappa))_{\mathbb{R}^3} = \frac{1}{\kappa^2}(\hat{H}_{\ell}^4(n), \hat{H}_{\ell}^4(m))_{\mathbb{R}^3}.
\]

Owing to (6.5) and (6.11) with \( \theta = \frac{1}{4} \), both the stiffness matrix \( S \) and the mass matrix \( M \) are tridiagonal. Consequently, the scheme (6.13) has an equivalent form in the following algebraic eigen-system:
\[
Su = \lambda_N Mu,
\] (6.15)

Interestingly, the matrix \( S + \frac{\kappa^2}{8} M \) is diagonal, so we can rewrite (6.15) as
\[
\left( S + \frac{\kappa^2}{8} M \right) u = \left( \lambda_N + \frac{\kappa^2}{8} \right) Mu,
\]
which leads to more efficient implementation.

In Figure 6.1, we plot the errors between the first 30 (counted by multiplicity) smallest numerical eigenvalues and exact eigenvalues in (6.7) 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 also affects the convergence rate.

6.2.2. 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
\[
\frac{q}{p} = \frac{2\nu - 2\mu}{\mu + 1} \quad \text{with} \quad \mu = 2p - 1 \in \mathbb{N}, \quad \nu = 2p + q - 1 \in \mathbb{N}_0.
\]

In the sequel, we consider the following Schrödinger equation with a fractional power potential as follows
\[
-\frac{1}{2} \Delta u(x) + Z|x|^{2q-2\mu} u(x) = \lambda u(x), \quad x \in \mathbb{R}^d,
\] (6.16)
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
\[
\mathcal{W}_{N,K}^{d,\frac{1}{\nu + \theta}} = \text{span}\{ \hat{\mathcal{H}}_{k,\ell}^{\frac{1}{\nu + \theta}, n}(\kappa x) : 0 \leq n \leq N, 1 \leq \ell \leq a_n^d, 0 \leq k \leq K, k, \ell, n \in \mathbb{N}_0 \}, \quad d \geq 2,
\]
and for \( d = 1 \), we can always assume \( \mu \) is odd and then define the approximation space as
\[
\mathcal{W}_{N,K}^{1,\frac{1}{\nu + \theta}} = \text{span}\{ \hat{\mathcal{H}}_{k,\ell}^{\frac{1}{\nu + \theta}, n}(\kappa x) : \frac{\mu + 1}{2} \delta_{n,0} \leq k \leq K, n = 0, 1 \},
\]
where \( \hat{\mathcal{H}}_{k,\ell}^{\frac{1}{\nu + \theta}, n} \) 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. Z1). This turns out important to deal with the strong singularities at the origin to ensure \( u(0) = 0 \) on one dimension.

The generalized Hermite spectral method for (6.2) is to find \( \lambda_{N,K} \in \mathbb{R} \) and \( u_{N,K} \in \mathcal{W}_{N,K}^{d,\frac{1}{\nu + \theta}} \setminus \{0\} \) such that
\[
\mathcal{B}(u_{N,K}, u_{N,K}) = \lambda_{N,K}(u_{N,K}, u_{N,K})_{\mathbb{R}^d}, \quad \forall u_{N,K} \in \mathcal{W}_{N,K}^{d,\frac{1}{\nu + \theta}}.
\]
In the implementation, we write
\[
u_{N,K}(x) = \sum_{n=0}^{N} \sum_{\ell=1}^{a_n^d} \sum_{k=0}^{K} \hat{u}_{\ell}^n \hat{\mathcal{H}}_{k,\ell}^{\frac{1}{\nu + \theta}, n}(\kappa x),
\]
and denote
\[
\hat{u}_{\ell}^n = (\hat{u}_{0,\ell}^n, \hat{u}_{1,\ell}^n, \ldots, \hat{u}_{a_n^d,\ell}^n)^t, \quad u = (\hat{u}_1^0, \hat{u}_2^0, \ldots, \hat{u}_{a_0^d,0}^0, \hat{u}_1^1, \hat{u}_2^1, \ldots, \hat{u}_{a_1^d,0}^1, \ldots, \hat{u}_1^N, \hat{u}_2^N, \ldots, \hat{u}_{a_N^d,0}^N)^t.
\]
The corresponding algebraic eigen-system of (6.17) is
\[
Su = \lambda_N Mu.
\]
In view of orthogonality (6.8) and (6.9), we find that for any \( q \in \mathbb{N}_0 \),
\[
(|x|^{\nu+1/\nu} \hat{\mathcal{H}}_{k,\ell}^{\frac{1}{\nu + \theta}, n}(\kappa)) \mathcal{B}(\hat{\mathcal{H}}_{k,\ell}^{\frac{1}{\nu + \theta}, n}, \hat{\mathcal{H}}_{j,\ell}^{\frac{1}{\nu + \theta}, m}(\kappa))_{\mathbb{R}^d} = \kappa^{-d} \mathcal{B}(\hat{\mathcal{H}}_{k,\ell}^{\frac{1}{\nu + \theta}, n}, \hat{\mathcal{H}}_{j,\ell}^{\frac{1}{\nu + \theta}, m})_{\mathbb{R}^d} = \frac{\mu + 1}{2} \kappa^{-d} c_{k,n}^{\frac{1}{\nu + \theta},d} c_{j,m}^{\frac{1}{\nu + \theta},d} \delta_{\ell \ell_0} \Gamma(k - p - q) \Gamma(p + \beta_n + q + 1) \Gamma(p + \beta_n + p + 1) \Gamma(-q)^2 (k - p)! (j - p)! (j - p)!^p.
\]
Furthermore, one has
\[
\mathcal{B}(\hat{\mathcal{H}}_{k,\ell}^{\frac{1}{\nu + \theta}, n}(\kappa), \hat{\mathcal{H}}_{j,\ell}^{\frac{1}{\nu + \theta}, m}(\kappa)) = \frac{1}{2} \kappa^{2-d} \mathcal{B}(\hat{\mathcal{H}}_{k,\ell}^{\frac{1}{\nu + \theta}, n}, \hat{\mathcal{H}}_{j,\ell}^{\frac{1}{\nu + \theta}, m})_{\mathbb{R}^d} + Z \kappa^{-2\nu+2d} \mathcal{B}(\hat{\mathcal{H}}_{k,\ell}^{\frac{1}{\nu + \theta}, n}, \hat{\mathcal{H}}_{j,\ell}^{\frac{1}{\nu + \theta}, m})_{\mathbb{R}^d}.
\]
These indicate that the stiffness matrix \( S \) is a banded matrix with a bandwidth \( \max(\nu, 1) \), and the mass matrix \( M \) is also banded with a bandwidth \( \mu \).

In the following tests, we fix \( N = 10 \), choose different scaling factor \( \kappa \) and test for different \( Z, \mu, \nu \) 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 6.2. Exponential orders of convergence are clearly observed in all cases, which demonstrate the effectiveness and outstanding performance of our Hermite spectral method.

7. Concluding remarks and acknowledgement

In this paper, we have introduced the following three families of GHFs in arbitrary \( d \) dimension, which are orthogonal in different sense as we tabulate below.
As direct applications, such basis functions have proven to be natural and optimal for Hermite approximation to, e.g., the integral fractional Laplacian and Schrödinger operators. Indeed, as we have always shown in the text, the related Hermite spectral methods have sparse and well-structured linear systems, and enjoy very high accuracy as the basis functions can be chosen to be tailored to the singularity of the kernel functions or solutions. Although we have only discussed two applications of this development, the ideas and tools can definitely be applied to many other problems of similar nature. We believe this work will be impactful in both theory and applications of spectral methods in unbounded domains.

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