

APPROXIMATION OF GAUSSIANS BY SPHERICAL GAUSS-LAGUERRE BASIS IN THE WEIGHED HILBERT SPACE

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ABSTRACT. This paper is devoted to the study of approximation of Gaussian functions by their partial Fourier sums of degree $N \in \mathbb{N}$ with respect to the spherical Gauss-Laguerre (SGL) basis in the weighted Hilbert space $L_2(\mathbb{R}^3, \omega_\lambda)$, where $\omega_\lambda(|\mathbf{x}|) = \exp(-|\mathbf{x}|^2/\lambda)$, $\lambda > 0$. We investigate the behaviour of the corresponding error of approximation with respect to the scale factor λ and degree of expansion N . As interim results we obtained formulas for the Fourier coefficients of Gaussians with respect to SGL basis in the space $L_2(\mathbb{R}^3, \omega_\lambda)$. Possible application of obtained results to the docking problem are described.

1. INTRODUCTION

Our goal in this paper is to study the behavior of the error of approximation of Gaussians by their partial Fourier sums with respect to the spherical Gauss-Laguerre (or shorter SGL) basis in the weighed Hilbert space $L_2(\mathbb{R}^3, \omega_\lambda)$, where $\omega_\lambda(|\mathbf{x}|) = \exp(-|\mathbf{x}|^2/\lambda)$, $\lambda > 0$, $\mathbf{x} = (x, y, z) \in \mathbb{R}^3$ and $|\mathbf{x}| = \sqrt{x^2 + y^2 + z^2}$. Motivation of our research comes from a wide range of applications of Gaussian functions in Life Sciences, in particular, in molecular modelling (see Section 5). The investigation of the behaviour of the Fourier coefficients of Gaussians with respect to SGL basis functions in the space $L_2(\mathbb{R}^3, \omega_\lambda)$ is of special interest to us.

By $\mathcal{H}^\lambda = \{H_{nlm}^\lambda : \mathbb{R}^3 \rightarrow \mathbb{C}, n \in \mathbb{N}, (l, m) \in \Delta_n\}$, where $\lambda > 0$ and $\Delta_n := \{(l, m) \in \mathbb{Z}^2 : l = \overline{0, n-1}, |m| = \overline{0, l}\}$, we denote the SGL basis (see Section 2 for details). For a function $f \in L_2(\mathbb{R}^3, \omega_\lambda)$ by $\mathcal{E}_N(f, \mathcal{H}^\lambda)$ we denote the error of approximation of this function by its partial Fourier sum of order $N \in \mathbb{N}$ with respect to the basis \mathcal{H}^λ in the space $L_2(\mathbb{R}^3, \omega_\lambda)$:

$$\mathcal{E}_N(f, \mathcal{H}^\lambda) := \left\| f - \sum_{n=1}^N \left(\sum_{(l,m) \in \Delta_n} \hat{f}_{nlm}^\lambda H_{nlm}^\lambda \right) \right\|_{L_2(\mathbb{R}^3, \omega_\lambda)},$$

where \hat{f}_{nlm}^λ are Fourier coefficients of the function f with respect to the basis \mathcal{H}^λ .

Our aim in this paper is to investigate the behaviour of the quantity $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ for the Gaussians $w(\mathbf{x} - \mathbf{x}_0) = \exp(-B|\mathbf{x} - \mathbf{x}_0|^2)$, where $B > 0$ is fixed and a point $\mathbf{x}_0 \in \mathbb{R}^3$ is given, with respect to the parameters $N \in \mathbb{N}$ and $\lambda > 0$.

Let us motivate our choice of basis. The SGL basis is constructed by using a separation-of-variables approach from the spherical harmonics and Laguerre polynomials. In the spherical coordinates

$$H_{nlm}^\lambda(r, \theta, \varphi) := R_{nl}^\lambda(r) Y_{lm}(\theta, \varphi),$$

2010 *Mathematics Subject Classification.* 33C05, 33C45, 33C55, 42C10.

Key words and phrases. Spherical harmonic, Laguerre polynomial, Gaussian, Hypergeometric function, Molecular docking.

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where the radial part $R_{nl}^\lambda(r)$ is defined via Laguerre polynomials, $\lambda > 0$ is a scale factor and the spherical part $Y_{lm}(\theta, \varphi)$ are the spherical harmonics.

By Δ_0 we denote the Laplace-Beltrami operator, i.e. the spherical part of the Laplace operator, that in spherical coordinates is given by

$$\Delta_0 = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}.$$

The spherical harmonics Y_{lm} are eigenfunctions of Δ_0 , i.e.

$$\Delta_0 Y_{lm}(\theta, \varphi) = -l(l+1)Y_{lm}(\theta, \varphi).$$

It is also known that spherical harmonics constitute an orthonormal basis of the space $L_2(\mathbb{S}^2)$ of square-integrable functions on the unit sphere \mathbb{S}^2 and are orthonormal in the sense that (see [5, chap. 1])

$$\int_0^{2\pi} \int_0^\pi Y_{lm}(\theta, \varphi) \overline{Y_{l'm'}(\theta, \varphi)} \sin \theta d\theta d\varphi = \delta_{ll'} \delta_{mm'}.$$

Because of described above properties of spherical harmonics they are important in many areas of science and are widely used as a shape descriptor (see, for example, [18]). On the other hand, the spherical harmonics are suitable for the approximation of smooth functions defined on the unit sphere \mathbb{S}^2 . Problems of linear and nonlinear approximation of Sobolev classes of smooth functions defined on \mathbb{S}^{d-1} , where d is the dimension of the space \mathbb{R}^d , by aggregates constructed by using spherical harmonics in the space $L_q(\mathbb{S}^{d-1})$, $1 \leq q \leq \infty$, are investigated by many authors, for instance, Kamzolov [10], Romanyuk [17], Dai and Xu [5] and Atkinson and Han [4]. From the viewpoint of practical applications in this paper we restrict ourselves to the case $d = 3$.

In order to obtain full sampling of the space \mathbb{R}^3 we use a radial function that extends spherical harmonics to polynomials in this space. Different choices of radial functions are possible. As Ritchie and Kemp [16] (see also [14]) we employ the radial part constructed by using associated Laguerre polynomials L_k^α , $k = 0, 1, \dots$ and $\alpha > 0$, that can be defined by the Rodrigues formula [7, p. 1051]

$$L_k^\alpha(t) = \frac{t^{-\alpha} \exp(t)}{k!} \frac{d^k (t^{k+\alpha} \exp(-t))}{dt^k}, \quad t \in \mathbb{R}.$$

Other radial functions such as Zernike polynomials may also be used (see papers [12] and [13] for details). Similar to the angular zeros of the spherical harmonics the Laguerre polynomials exhibit radial zeros and they are orthogonal with respect to a weight factor $t^\alpha \exp(-t)$, i.e.

$$\int_0^\infty L_k^{(\alpha)}(t) L_{k'}^{(\alpha)}(t) t^\alpha \exp(-t) dt = \frac{\Gamma(k + \alpha + 1)}{k!} \delta_{kk'}.$$

Let us sketch the main results of the paper. The basic ingredient to investigate the behaviour of the quantity $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ is to use the Parseval's equality and representation formulas for the SGL Fourier coefficients that we also obtain in this paper (see Section 3 and 4 for details).

At first we consider the function $w(\mathbf{x} - \mathbf{x}_0) = \exp(-B|\mathbf{x} - \mathbf{x}_0|^2)$ in the case when $\mathbf{x}_0 = \mathbf{0}$. For the quantity $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ we have that

$$(1.1) \quad \mathcal{E}_N(w, \mathcal{H}^\lambda) = \sqrt{\frac{2\pi\Gamma(N+3/2)}{\Gamma(N+1)}} \frac{\lambda^{3/4}}{(1+B\lambda)^{3/2}} \left(\frac{B\lambda}{1+B\lambda}\right)^N \times \sqrt{{}_2F_1\left(1, N+3/2, N+1; \left(\frac{B\lambda}{1+B\lambda}\right)^2\right)},$$

where Γ is the gamma function and ${}_2F_1$ is the hypergeometric function (see the end of this section for a definition).

For $N \rightarrow \infty$ the asymptotic behaviour of this quantity is described by (see Figure 1, left)

$$(1.2) \quad \mathcal{E}_N(w, \mathcal{H}^\lambda) \sim C(\lambda, B)(N+1)^{1/4} \left(\frac{B\lambda}{1+B\lambda}\right)^N,$$

where the constant $C(\lambda, B)$ can be estimated as follows

$$C(\lambda, B) = \frac{\sqrt{2\pi}\lambda^{3/4}}{(1+B\lambda)^{3/2}} c(\lambda, B)$$

and

$$\frac{1+B\lambda}{\sqrt{1+2B\lambda}} < c(\lambda, B) \leq \left(\frac{2}{3} \cdot \frac{(1+B\lambda)^3 - (1+2B\lambda)^{3/2}}{(B\lambda)^2\sqrt{1+2B\lambda}}\right)^{1/2} \cdot \frac{1+B\lambda}{\sqrt{1+2B\lambda}}.$$

With respect to the parameter λ the quantity $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ is increasing on the segment $(0, +\infty)$ for all fixed $N \in \mathbb{N}$. Moreover, for all $N \in \mathbb{N}$ (see Figure 1, right)

$$(1.3) \quad \lim_{\lambda \rightarrow \infty} \mathcal{E}_N(w, \mathcal{H}^\lambda) = \left(\frac{\pi}{2B}\right)^{3/4}.$$

For the function $w(\mathbf{x} - \mathbf{x}_0) = \exp(-B|\mathbf{x} - \mathbf{x}_0|^2)$ where $\mathbf{x}_0 \neq 0$ we have numerical evidence of the fact that the quantity $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ keeps its behaviour with respect to the parameter $\lambda > 0$ when a point \mathbf{x}_0 is shifted from the origin. Unfortunately, due to complex form of the SGL Fourier coefficients of Gaussians $w(\mathbf{x} - \mathbf{x}_0)$ in case $\mathbf{x}_0 \neq 0$, we do not have an analytical proof of this effect (see Section 4 for details). Note that with respect to $N \in \mathbb{N}$ it is easily seen from the Parseval's equality that $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ decays with respect to N , i.e. $\mathcal{E}_N(w, \mathcal{H}^\lambda) \geq \mathcal{E}_{N+1}(w, \mathcal{H}^\lambda)$ for all $N \in \mathbb{N}$.

The present paper has the following structure. In Section 2 we give the main definitions that are used in the paper. Section 3 contains a proof of the relations (1.1), (1.2) and (1.3) as well as formulas for the SGL Fourier coefficients for the function $w(\mathbf{x}) = \exp(-B|\mathbf{x}|^2)$. In Section 4 we obtain formulas for the SGL Fourier coefficients of the functions $w(\mathbf{x} - \mathbf{x}_0) = \exp(-B|\mathbf{x} - \mathbf{x}_0|^2)$ in case when $\mathbf{x}_0 \neq 0$ and show numerical results with respect to the behaviour of the quantity $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ for these functions. In Section 5 we describe one possible application of obtained results to the molecular docking problem.

Notation. As usual $\mathbb{N} = \{1, 2, 3, \dots\}$, \mathbb{R} and \mathbb{C} denote the natural, real and complex numbers, respectively. Consequently, \mathbb{R}^3 is the set of all vectors $\mathbf{x} = (x, y, z)$ and $|\mathbf{x}| = \sqrt{x^2 + y^2 + z^2}$ is the Euclidean norm of a vector \mathbf{x} . Letters C_i , $i = 1, 2, \dots$, denote positive constants. We indicate in brackets dependency on some parameters. Let $(t)_n = \frac{\Gamma(t+n)}{\Gamma(t)}$, $n \in \mathbb{N}$, and $(t)_0 = 1$

be the Pochhammer symbol [2, p. 256], where Γ is the gamma function. By ${}_2F_1$ we denote the hypergeometric function [7, §9.1]

$$(1.4) \quad {}_2F_1(a, b, c, t) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{(c)_n} \frac{t^n}{n!}, \quad |t| < 1.$$

Further for given functions f and g we use the binary relation $f(t) \sim g(t)$ as $t \rightarrow \infty$ if and only if $\lim_{t \rightarrow \infty} \frac{f(t)}{g(t)} = 1$. The symbol δ_{ij} is the Kronecker delta and as usual $\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j, \\ 1 & \text{if } i = j. \end{cases}$

2. PRELIMINARIES

As stated in the introduction the main goal of this paper is to investigate the behavior of the error of approximation of Gaussians by their partial Fourier sums with respect to the spherical Gauss-Laguerre (or SGL) basis in the weighed Hilbert space $L_2(\mathbb{R}^3, \omega_\lambda)$. In this section we present the main definitions.

By $L_2(\mathbb{R}^3, \omega_\lambda)$, where $\omega_\lambda(|\mathbf{x}|) = \exp(-|\mathbf{x}|^2/\lambda)$, $\mathbf{x} \in \mathbb{R}^3$ and $\lambda > 0$, we denote the weighted Hilbert space

$$L_2(\mathbb{R}^3, \omega_\lambda) := \left\{ f : \mathbb{R}^3 \rightarrow \mathbb{C}, \int_{\mathbb{R}^3} |f(\mathbf{x})|^2 \omega_\lambda(|\mathbf{x}|) d\mathbf{x} < \infty \right\}.$$

The inner product in this space is defined as

$$(2.1) \quad \langle f, g \rangle_{L_2(\mathbb{R}^3, \omega_\lambda)} := \int_{\mathbb{R}^3} f(\mathbf{x}) \overline{g(\mathbf{x})} \omega_\lambda(|\mathbf{x}|) d\mathbf{x}, \quad f, g \in L_2(\mathbb{R}^3, \omega_\lambda)$$

and the norm as

$$\|f\|_{L_2(\mathbb{R}^3, \omega_\lambda)} := \sqrt{\langle f, f \rangle_{L_2(\mathbb{R}^3, \omega_\lambda)}}, \quad f \in L_2(\mathbb{R}^3, \omega_\lambda).$$

Further we define the SGL basis functions. For this end we use the spherical coordinates (r, θ, φ) , where $r \in [0, \infty)$ is the radius, $\theta \in [0, \pi]$ is the polar angle, $\varphi \in [0, 2\pi)$ is the azimuthal angle, to write the Cartesian coordinates x , y and z as

$$\begin{aligned} x &= r \sin \theta \cos \varphi, \\ y &= r \sin \theta \sin \varphi, \\ z &= r \cos \theta. \end{aligned}$$

In the following we write $f(\mathbf{x}) = f(r, \theta, \varphi)$ if (r, θ, φ) are spherical coordinates of the point $\mathbf{x} = (x, y, z)$, in which case we simply write $\mathbf{x} = (r, \theta, \varphi)$.

Then the inner product (2.1) can be rewritten as

$$\langle f, g \rangle_{L_2(\mathbb{R}^3, \omega_\lambda)} := \int_0^\infty \int_0^\pi \int_0^{2\pi} f(r, \theta, \varphi) \overline{g(r, \theta, \varphi)} \omega_\lambda(r) r^2 \sin \theta d\varphi d\theta dr, \quad f, g \in L_2(\mathbb{R}^3, \omega_\lambda),$$

where $r^2 \sin \theta$ is the Jacobian of the transform from Cartesian to spherical coordinates.

Let Δ_n be the following set of indices $\Delta_n = \{(l, m) \in \mathbb{Z}^2 : l = 0, \dots, n-1, |m| = 0, \dots, l\}$. For $\lambda > 0$ by $\mathcal{H}^\lambda = \{H_{nlm}^\lambda : \mathbb{R}^3 \rightarrow \mathbb{C}, n \in \mathbb{N}, (l, m) \in \Delta_n\}$ we denote the system of functions

$$H_{nlm}^\lambda(r, \theta, \varphi) := R_{nl}^\lambda(r) Y_{lm}(\theta, \varphi),$$

where the radial part R_{nl}^λ is defined as

$$R_{nl}^\lambda(r) = \left(\frac{2(n-l-1)!}{\lambda^{3/2}\Gamma(n+1/2)} \right)^{1/2} (r/\sqrt{\lambda})^l L_{n-l-1}^{(l+1/2)}(r^2/\lambda),$$

with associated Laguerre polynomials L_k^α and a scale factor $\lambda > 0$. The spherical part Y_{lm} is represented by spherical harmonics that is given by

$$Y_{lm}(\theta, \varphi) = \left(\frac{(2l+1)(l-m)!}{4\pi(l+m)!} \right)^{1/2} P_{lm}(\cos \theta) \exp(im\varphi),$$

where $P_{lm}(t) = \frac{(-1)^m}{2^l l!} (1-t^2)^{m/2} \frac{d^{l+m}}{dt^{l+m}} (t^2-1)^l$ are associated Legendre polynomials. Note that in the case $m=0$ we simply write P_l instead of P_{l0} .

By $\widehat{f}_{nlm}^\lambda$ we denote the Fourier coefficients of the function $f \in L_2(\mathbb{R}^3, \omega_\lambda)$ with respect to the system \mathcal{H}^λ , i.e.

$$\widehat{f}_{nlm}^\lambda = \int_0^\infty \int_0^\pi \int_0^{2\pi} f(r, \theta, \varphi) \overline{H_{nlm}^\lambda(r, \theta, \varphi)} \omega_\lambda(r) r^2 \sin \theta \, d\varphi \, d\theta \, dr.$$

The following theorem holds.

Theorem 2.1. [14] *The system \mathcal{H}^λ constitutes an orthonormal basis in the space $L_2(\mathbb{R}^3, \omega_\lambda)$, i.e. each function $f \in L_2(\mathbb{R}^3, \omega_\lambda)$ can be uniquely decomposed into the series*

$$f = \sum_{n=1}^{\infty} \left(\sum_{(l,m) \in \Delta_n} \widehat{f}_{nlm}^\lambda H_{nlm}^\lambda \right)$$

with convergence in the sense of the space $L_2(\mathbb{R}^3, \omega_\lambda)$.

Note, that although the authors in [14] consider only the case $\lambda = 1$, the scale factor λ does not influence on orthogonality and completeness of the system \mathcal{H}^λ .

As was mentioned in the introduction, the basis \mathcal{H}^λ is called a spherical Gauss-Laguerre basis or shorter SGL basis and the coefficients $\widehat{f}_{nlm}^\lambda$ are called SGL Fourier coefficients of the function f . More detailed information about this basis can be found in [14] and [15].

3. APPROXIMATION OF THE FUNCTION $\exp(-B|\mathbf{x}|^2)$ IN THE SPACE $L_2(\mathbb{R}^3, \omega_\lambda)$

In this section we investigate the behaviour of the quantity $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ where $w(\mathbf{x}) = \exp(-B|\mathbf{x}|^2)$ with respect to the parameters $N \in \mathbb{N}$ and $\lambda > 0$.

At first we formulate results regarding the SGL Fourier coefficients of the function w .

Theorem 3.1. *The SGL Fourier coefficients of the function $w(\mathbf{x}) = \exp(-B|\mathbf{x}|^2)$, $\mathbf{x} \in \mathbb{R}^3$, $B > 0$, can be written as*

$$(3.1) \quad \widehat{w}_{n00}^\lambda = \sqrt{\frac{2\pi\Gamma(n+1/2)}{\Gamma(n)}} \frac{\lambda^{3/4}}{(1+B\lambda)^{3/2}} \left(\frac{B\lambda}{1+B\lambda} \right)^{n-1}, \quad \lambda > 0,$$

and $\widehat{w}_{nlm}^\lambda = 0$ for $l \neq 0$, $m \neq 0$.

Proof. With $w(\mathbf{x}) = w(r, \theta, \varphi) = \exp(-Br^2)$ we obtain

$$\begin{aligned}\widehat{w}_{nlm}^\lambda &= \int_0^\infty \int_0^\pi \int_0^{2\pi} \exp(-Br^2) \overline{H_{nlm}^\lambda(r, \theta, \varphi)} \exp(-r^2/\lambda) r^2 \sin \theta \, d\varphi \, d\theta \, dr \\ &= \int_0^\infty \int_0^\pi \int_0^{2\pi} \exp(-Br^2) R_{nl}^\lambda(r) \overline{Y_{lm}(\theta, \varphi)} \exp(-r^2/\lambda) r^2 \sin \theta \, d\varphi \, d\theta \, dr.\end{aligned}$$

Since

$$\int_0^\pi \int_0^{2\pi} \overline{Y_{lm}(\theta, \varphi)} \sin \theta \, d\varphi \, d\theta = \begin{cases} 2\sqrt{\pi}, & m = l = 0, \\ 0, & \text{otherwise,} \end{cases}$$

we have that $w_{nlm}^\lambda = 0$ if $l \neq 0$, $m \neq 0$.

Let now $n \in \mathbb{N}$ and $l = m = 0$. Making change of variables two times ($r/\sqrt{\lambda} \rightarrow t$ and $t^2 \rightarrow y$) we get

$$\begin{aligned}\left(\frac{8\pi(n-1)!}{\lambda^{3/2}\Gamma(n+1/2)}\right)^{-1/2} \widehat{w}_{n00}^\lambda &= \int_0^\infty \exp(-Br^2) L_{n-1}^{1/2}(r^2/\lambda) \exp(-r^2/\lambda) r^2 \, dr \\ &= \lambda^{3/2} \int_0^\infty \exp(-t^2(1+B\lambda)) L_{n-1}^{1/2}(t^2) t^2 \, dt \\ &= \frac{1}{2} \lambda^{3/2} \int_0^\infty \exp(-y(1+B\lambda)) L_{n-1}^{1/2}(y) y^{1/2} \, dy.\end{aligned}$$

Using formula [7, 7.414 (7)] for $\beta > -1$ and $s > 0$

$$\int_0^\infty \exp(-st) t^\beta L_n^{(\alpha)}(t) \, dt = \frac{\Gamma(\beta+1) \Gamma(\alpha+n+1)}{n! \Gamma(\alpha+1)} s^{-\beta-1} {}_2F_1(-n, \beta+1, \alpha+1, 1/s),$$

where ${}_2F_1$ is the hypergeometric function, we obtain

$$\widehat{w}_{n00}^\lambda = \sqrt{\frac{2\pi\Gamma(n+1/2)}{(n-1)!}} \frac{\lambda^{3/4}}{(1+B\lambda)^{3/2}} {}_2F_1\left(-n+1, \frac{3}{2}, \frac{3}{2}, \frac{1}{1+B\lambda}\right).$$

From the following property of the hypergeometric function ${}_2F_1$ [2, p. 556]

$${}_2F_1(a, c, c, b) = (1-b)^{-a},$$

we get that

$$\widehat{w}_{n00}^\lambda = \sqrt{\frac{2\pi\Gamma(n+1/2)}{(n-1)!}} \frac{\lambda^{3/4}}{(1+B\lambda)^{3/2}} \left(1 - \frac{1}{1+B\lambda}\right)^{n-1}.$$

By using simple transformations and the definition of the Gamma function we obtain the desired formula (3.1). \square

Note that we can derive the asymptotic behaviour of the coefficients $\widehat{w}_{n00}^\lambda$ when $n \rightarrow \infty$ and λ is fixed and vice versa when $\lambda \rightarrow \infty$ and n is fixed.

Let at first $\lambda > 0$ be fixed. According to the expansion (4.15) from [6] the quantity $\frac{\Gamma(n+1/2)}{\Gamma(n)}$ behaves for $n \rightarrow \infty$ as

$$(3.2) \quad \frac{\Gamma(n+1/2)}{\Gamma(n)} \sim n^{1/2}.$$

From this we have that

$$\widehat{w}_{n00}^\lambda \sim C_1(\lambda, B)n^{1/4} \left(\frac{B\lambda}{1+B\lambda} \right)^{n-1}, \quad n \rightarrow \infty,$$

where $C_1(\lambda, B) = \frac{\sqrt{2\pi}\lambda^{3/4}}{(1+B\lambda)^{3/2}}$.

Let now $n \in \mathbb{N}$ be fixed and $\lambda \rightarrow \infty$. From (3.1) it is easy to see that in this case

$$\widehat{w}_{n00}^\lambda \sim C_2(n, B)\lambda^{-3/4},$$

where $C_2(n, B) = B^{-3/4} \sqrt{\frac{2\pi\Gamma(n+1/2)}{\Gamma(n)}}$.

Now we are ready to prove the following result on the error of approximation $\mathcal{E}_N(w, \mathcal{H}^\lambda)$.

Theorem 3.2. *For the function $w(\mathbf{x}) = e^{-B|\mathbf{x}|^2}$, $\mathbf{x} \in \mathbb{R}^3$, $B > 0$, and $\lambda > 0$, $N \in \mathbb{N}$, we have*

$$\begin{aligned} \mathcal{E}_N(w, \mathcal{H}^\lambda) &= \sqrt{\frac{2\pi\Gamma(N+3/2)}{\Gamma(N+1)} \frac{\lambda^{3/4}}{(1+B\lambda)^{3/2}} \left(\frac{B\lambda}{1+B\lambda} \right)^N} \\ &\quad \times \sqrt{{}_2F_1 \left(1, N+3/2, N+1; \left(\frac{B\lambda}{1+B\lambda} \right)^2 \right)}. \end{aligned}$$

Proof. Applying the Parseval's equality we obtain

$$(3.3) \quad \begin{aligned} \mathcal{E}_N^2(w, \mathcal{H}^\lambda) &= \left\| w - \sum_{n=1}^N \left(\sum_{(l,m) \in \Delta_n} \widehat{w}_{nlm}^\lambda H_{nlm}^\lambda \right) \right\|_{L_2(\mathbb{R}^3, \omega_\lambda)}^2 \\ &= \sum_{n=N+1}^{\infty} \left(\sum_{(l,m) \in \Delta_n} |\widehat{w}_{nlm}^\lambda|^2 \right). \end{aligned}$$

Substituting the SGL Fourier coefficients (3.1) in (3.3) we get

$$\begin{aligned} \mathcal{E}_N^2(w, \mathcal{H}^\lambda) &= \sum_{n=N+1}^{\infty} |\widehat{w}_{n00}^\lambda|^2 = 2\pi \left(\frac{\lambda^{3/4}}{(1+B\lambda)^{3/2}} \right)^2 \sum_{n=N+1}^{\infty} \frac{\Gamma(n+1/2)}{\Gamma(n)} \left(\frac{B\lambda}{1+B\lambda} \right)^{2(n-1)} \\ &= 2\pi \left(\frac{\lambda^{3/4}}{(1+B\lambda)^{3/2}} \right)^2 \left(\frac{B\lambda}{1+B\lambda} \right)^{2N} \sum_{k=0}^{\infty} \frac{\Gamma(k+N+3/2)}{\Gamma(k+N+1)} \left(\frac{B\lambda}{1+B\lambda} \right)^{2k}. \end{aligned}$$

Using the expansion of the hypergeometric function ${}_2F_1$ (1.4)

$$(3.4) \quad \sum_{k=0}^{\infty} \frac{\Gamma(k+a)}{\Gamma(k+b)} x^k = \frac{\Gamma(a)}{\Gamma(b)} {}_2F_1(1, a, b; x), \quad |x| < 1,$$

we obtain the necessary equality. □

Before coming to the next theorem we give a proof of one property of the hypergeometric function that we further use few times. Let

$$\mathbf{B}_z(a, b) = \int_0^z t^{a-1}(1-t)^{b-1} dt, \quad a, b > 0, |z| < 1,$$

be the incomplete beta function [7, 8.39]. By using transformation formulas for the hypergeometric function ${}_2F_1$ [7, 9.131]

$$(3.5) \quad {}_2F_1(a, b, c; t) = (1-t)^{c-b-a} {}_2F_1(c-a, c-b, c; t),$$

we obtain

$${}_2F_1(1, b, c; t) = (1-t)^{c-b-1} {}_2F_1(c-1, c-b, c; t).$$

Applying the following formula [7, 8.391]

$${}_2F_1(p, 1-q, p+1; t) = pt^{-p} \mathbf{B}_t(p, q)$$

with $p = c-1$ and $q = b-c+1$, we get

$${}_2F_1(1, b, c; t) = (c-1)t^{1-c}(1-t)^{c-b-1} \mathbf{B}_t(c-1, b-c+1).$$

Finally, from [2, 6.6.2] and [2, 26.5.6] we have

$$\mathbf{B}_t(n, \beta) = \mathbf{B}(n, \beta) - (1-t)^\beta \sum_{k=0}^{n-1} \frac{(-1)^k (n-1)!}{k!(n-1-k)!} \frac{(1-t)^k}{\beta+k}, \quad n \in \mathbb{N},$$

where $\mathbf{B}(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}$ is the beta function [7, 8.384 (1)], which implies

$$(3.6) \quad \begin{aligned} {}_2F_1(1, b, c; t) &= \frac{\Gamma(c)\Gamma(b-c+1)}{\Gamma(b)} t^{1-c}(1-t)^{c-b-1} \\ &\quad - t^{1-c} \sum_{k=0}^{c-2} \frac{(-1)^k (c-1)!}{k!(c-2-k)!} \frac{(1-t)^k}{b-c+1+k}, \end{aligned}$$

for $c \in \mathbb{N}$ and $0 < t < 1$.

The next theorem describes the asymptotic behaviour of the quantity $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ with respect to the parameter $N \in \mathbb{N}$ for fixed $\lambda, B > 0$ (see Figure 1, left).

Theorem 3.3. *The quantity $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ for $w(\mathbf{x}) = \exp(-B|\mathbf{x}|^2)$, $B, \lambda > 0$, asymptotically behaves like*

$$(3.7) \quad \mathcal{E}_N(w, \mathcal{H}^\lambda) \sim C_3(\lambda, B)(N+1)^{1/4} \left(\frac{B\lambda}{1+B\lambda} \right)^N, \quad N \rightarrow \infty,$$

where $C_3(\lambda, B) = \frac{\sqrt{2\pi}\lambda^{3/4}}{(1+B\lambda)^{3/2}} C_4(\lambda, B)$ and

$$\frac{1+B\lambda}{\sqrt{1+2B\lambda}} < C_4(\lambda, B) \leq \sqrt{\frac{2}{3} \cdot \frac{(1+B\lambda)^3 - (1+2B\lambda)^{3/2}}{(B\lambda)^2 \sqrt{1+2B\lambda}}} \cdot \frac{1+B\lambda}{\sqrt{1+2B\lambda}}.$$

Proof. To prove the asymptotic formula (3.7) we use Theorem 3.2 together with (3.2) and property of boundeness of the function ${}_2F_1\left(1, N+3/2, N+1; \left(\frac{B\lambda}{1+B\lambda}\right)^2\right)$ with respect to the parameter N that we show below.

From (3.2) we have

$$(3.8) \quad \sqrt{\frac{\Gamma(N+3/2)}{\Gamma(N+1)}} \sim (N+1)^{1/4}, \quad N \rightarrow \infty.$$

Let us further prove that ${}_2F_1\left(1, N+3/2, N+1; \left(\frac{B\lambda}{1+B\lambda}\right)^2\right)$ is bounded with respect to $N \in \mathbb{N}$ for all fixed positive values B and λ . For an arbitrary $N \in \mathbb{N}$ we consider a sequence $a_N := {}_2F_1(1, N+3/2, N+1; t)$, $0 < t < 1$ and prove that $a_N > a_{N+1}$ for all $N \in \mathbb{N}$.

According to (3.4) we obtain

$$\begin{aligned} a_N - a_{N+1} &= {}_2F_1(1, N+3/2, N+1; t) - {}_2F_1(1, N+5/2, N+2; t) \\ &= \frac{\Gamma(N+1)}{\Gamma(N+3/2)} \sum_{k=0}^{\infty} \frac{\Gamma(k+N+3/2)}{\Gamma(k+N+1)} t^k - \frac{\Gamma(N+2)}{\Gamma(N+5/2)} \sum_{k=0}^{\infty} \frac{\Gamma(k+N+5/2)}{\Gamma(k+N+2)} t^k. \end{aligned}$$

Let us denote $f(N) = \frac{\Gamma(N+5/2)}{\Gamma(N+1)}(a_N - a_{N+1})$, then

$$f(N) = \frac{\Gamma(N+5/2)}{\Gamma(N+3/2)} \sum_{k=0}^{\infty} \frac{\Gamma(k+N+3/2)}{\Gamma(k+N+1)} t^k - \frac{\Gamma(N+2)}{\Gamma(N+1)} \sum_{k=0}^{\infty} \frac{\Gamma(k+N+5/2)}{\Gamma(k+N+2)} t^k.$$

Further we need the following properties of the Gamma function

$$(3.9) \quad \frac{\Gamma(N+3/2)}{\Gamma(N+5/2)} = \frac{2}{2N+3}.$$

By using last equality we get

$$\begin{aligned} f(N) &= \frac{2N+3}{2} \sum_{k=0}^{\infty} \frac{\Gamma(k+N+3/2)}{\Gamma(k+N+1)} t^k - (N+1) \sum_{k=0}^{\infty} \frac{\Gamma(k+N+5/2)}{\Gamma(k+N+2)} t^k \\ &= \sum_{k=0}^{\infty} \frac{\Gamma(k+N+5/2)}{\Gamma(k+N+1)} \left((N+3/2) \frac{\Gamma(k+N+3/2)}{\Gamma(k+N+5/2)} - (N+1) \frac{\Gamma(k+N+1)}{\Gamma(k+N+2)} \right) t^k \\ &= \sum_{k=0}^{\infty} \frac{\Gamma(k+N+5/2)}{\Gamma(k+N+1)} \frac{k t^k}{(2N+3+2k)(N+1+k)}, \end{aligned}$$

which implies that $f(N) > 0$ and consequently $a_N > a_{N+1}$, $N \in \mathbb{N}$. From this for all $N \in \mathbb{N}$ we have

$$(3.10) \quad \begin{aligned} {}_2F_1\left(1, N+3/2, N+1; \left(\frac{B\lambda}{1+B\lambda}\right)^2\right) &\leq {}_2F_1\left(1, 5/2, 2; \left(\frac{B\lambda}{1+B\lambda}\right)^2\right) \\ &= \frac{2}{3} \cdot \frac{(1+B\lambda)^3 - (1+2B\lambda)^{3/2}}{(B\lambda)^2 \sqrt{1+2B\lambda}} \cdot \frac{(1+B\lambda)^2}{1+2B\lambda}. \end{aligned}$$

The last equality is due to (3.6). On the other hand, by using

$$\Gamma(n+1/2) = \frac{(2n)!}{4^n n!} \sqrt{\pi}, \quad n \in \mathbb{N},$$

we get

$$\begin{aligned}
{}_2F_1\left(1, N + 3/2, N + 1; \left(\frac{B\lambda}{1 + B\lambda}\right)^2\right) &= \frac{\Gamma(N + 1)}{\Gamma(N + 3/2)} \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 1)} \left(\frac{B\lambda}{1 + B\lambda}\right)^{2k} \\
&= 1 + \sum_{k=1}^{\infty} \frac{(2N + 2k + 1)!!}{(2N + 2k)!!} \left(\frac{B\lambda}{1 + B\lambda}\right)^{2k} \\
(3.11) \qquad &> \sum_{k=0}^{\infty} \left(\frac{B\lambda}{1 + B\lambda}\right)^{2k} = \frac{(1 + B\lambda)^2}{1 + 2B\lambda}.
\end{aligned}$$

From (3.10) and (3.11) we have that for all $N \in \mathbb{N}$

$$(3.12) \qquad \frac{(1 + B\lambda)^2}{1 + 2B\lambda} < C_4^2(\lambda, B) \leq \frac{2}{3} \cdot \frac{(1 + B\lambda)^3 - (1 + 2B\lambda)^{3/2}}{(B\lambda)^2 \sqrt{1 + 2B\lambda}} \cdot \frac{(1 + B\lambda)^2}{1 + 2B\lambda}.$$

From relations (3.8), (3.12) and Theorem 3.2 we get the asymptotic formula (3.7). \square

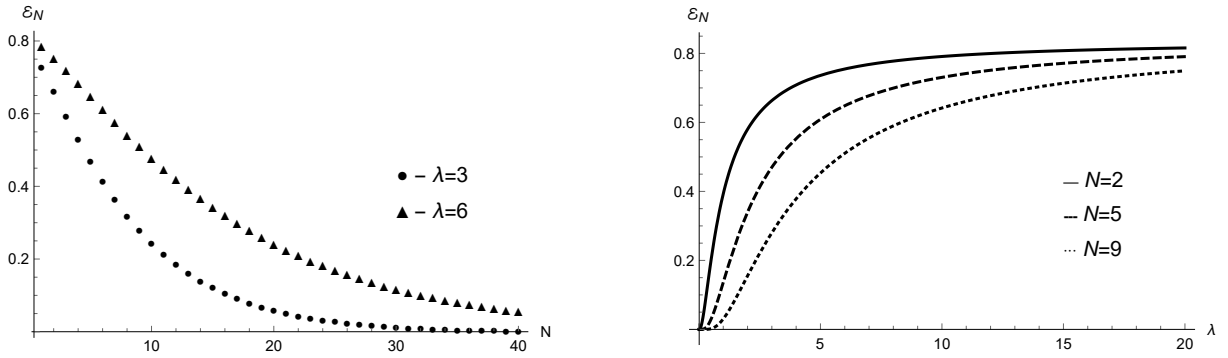


FIGURE 1. Graphics of the behavior of $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ ($B = 2$) with respect to N (left) and with respect to λ (right).

The next theorem describes the behaviour of the quantity $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ with respect to the parameter $\lambda > 0$ for fixed $N \in \mathbb{N}$ and $B > 0$ (see Figure 1, right).

Theorem 3.4. *The quantity $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ for $w(\mathbf{x}) = \exp(-B|\mathbf{x}|^2)$, as a function of λ , $\lambda > 0$, is increasing on the segment $(0, +\infty)$ for all $N \in \mathbb{N}$. Moreover,*

$$(3.13) \qquad \lim_{\lambda \rightarrow \infty} \mathcal{E}_N(w, \mathcal{H}^\lambda) = \left(\frac{\pi}{2B}\right)^{3/4}, \quad N \in \mathbb{N}.$$

Proof. At first we prove (3.13). Let us consider

$$(3.14) \qquad J := \lim_{\lambda \rightarrow \infty} \frac{\lambda^{3/2}}{(1 + B\lambda)^3} {}_2F_1\left(1, N + 3/2, N + 1; \left(\frac{B\lambda}{1 + B\lambda}\right)^2\right).$$

For this end we use the following limit (see Theorem 2.1.3 [3, p. 63])

$$(3.15) \qquad \lim_{z \rightarrow 1} (1 - z)^{a+b-c} {}_2F_1(a, b, c; z) = \frac{\Gamma(c)\Gamma(a + b - c)}{\Gamma(a)\Gamma(b)}, \quad c - b - a < 0.$$

From (3.15) taking into account that $\left(\frac{B\lambda}{1+B\lambda}\right)^2 \rightarrow 1$ as $\lambda \rightarrow \infty$ we have

$$(3.16) \quad \lim_{\lambda \rightarrow \infty} \left(1 - \left(\frac{B\lambda}{1+B\lambda}\right)^2\right)^{\frac{3}{2}} {}_2F_1\left(1, N + 3/2, N + 1; \left(\frac{B\lambda}{1+B\lambda}\right)^2\right) = \frac{\Gamma(N+1)\Gamma(3/2)}{\Gamma(N+3/2)}.$$

By using (3.16) we get for (3.14)

$$(3.17) \quad \begin{aligned} J &= \lim_{\lambda \rightarrow \infty} \frac{\lambda^{3/2}}{(1+B\lambda)^3} \left(1 - \left(\frac{B\lambda}{1+B\lambda}\right)^2\right)^{-3/2} \\ &\quad \times \left(1 - \left(\frac{B\lambda}{1+B\lambda}\right)^2\right)^{3/2} {}_2F_1\left(1, N + 3/2, N + 1; \left(\frac{B\lambda}{1+B\lambda}\right)^2\right) \\ &= \frac{\Gamma(N+1)\Gamma(3/2)}{\Gamma(N+3/2)} \lim_{\lambda \rightarrow \infty} \frac{\lambda^{3/2}}{(1+2B\lambda)^{3/2}} = \frac{\Gamma(N+1)\Gamma(3/2)}{\Gamma(N+3/2)} \left(\frac{1}{2B}\right)^{3/2}. \end{aligned}$$

From (3.14), (3.17) and Theorem 3.2, using that $\Gamma(3/2) = \frac{1}{2}\sqrt{\pi}$, we obtain

$$\lim_{\lambda \rightarrow \infty} \mathcal{E}_N(w, \mathcal{H}^\lambda) = \sqrt{\frac{2\pi\Gamma(N+3/2)}{\Gamma(N+1)}} \sqrt{\frac{\Gamma(N+1)\Gamma(3/2)}{\Gamma(N+3/2)}} \left(\frac{1}{2B}\right)^{3/4} = \left(\frac{\pi}{2B}\right)^{3/4},$$

for all $N \in \mathbb{N}$.

Our further goal is to prove that $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ is increasing for $\lambda \in (0; +\infty)$. Let us first find $\frac{\partial(\mathcal{E}_N(w, \mathcal{H}^\lambda))}{\partial\lambda}$. Note that the derivative of the hypergeometric function ${}_2F_1$ is given by the formula [2, 15.2.1]

$$\frac{\partial({}_2F_1(a, b, c; x))}{\partial x} = \frac{ab}{c} {}_2F_1(a+1, b+1, c+1; x).$$

Taking this into account we get

$$\begin{aligned} \frac{\partial(\mathcal{E}_N(w, \mathcal{H}^\lambda))}{\partial\lambda} &= \sqrt{\frac{2\pi\Gamma(N+3/2)}{\Gamma(N+1)}} \left(\frac{B\lambda}{1+B\lambda}\right)^{N-1} \\ &\quad \times \frac{B\lambda^{3/4} \times R(N, \lambda)}{4(1+B\lambda)^{7/2} \sqrt{{}_2F_1\left(1, N + 3/2, N + 1; \left(\frac{B\lambda}{1+B\lambda}\right)^2\right)}}, \end{aligned}$$

where

$$\begin{aligned} R(N, \lambda) &:= (3 + 4N - 3B\lambda) {}_2F_1\left(1, N + 3/2, N + 1; \left(\frac{B\lambda}{1+B\lambda}\right)^2\right) \\ &\quad + 4 \left(\frac{B\lambda}{1+B\lambda}\right)^2 \frac{N+3/2}{N+1} {}_2F_1\left(2, N + 5/2, N + 2; \left(\frac{B\lambda}{1+B\lambda}\right)^2\right), \end{aligned}$$

and we prove that $R(N, \lambda) > 0$ for $\lambda > 0$ and all choices of parameters N and B .

For simplicity we denote $\frac{B\lambda}{1+B\lambda} = t$. Then

$$(3.18) \quad \begin{aligned} R(N, t) &= \left(3 + 4N - \frac{3t}{1-t}\right) {}_2F_1(1, N + 3/2, N + 1; t^2) \\ &\quad + 4t^2 \frac{N+3/2}{N+1} {}_2F_1(2, N + 5/2, N + 2; t^2). \end{aligned}$$

By using the following expansions of the hypergeometric functions

$$\begin{aligned}
{}_2F_1(2, N + 5/2, N + 2; t^2) &= \sum_{k=0}^{\infty} \frac{(2)_k (N + 5/2)_k}{(N + 2)_k k!} t^{2k} \\
&= \frac{\Gamma(N + 2)}{\Gamma(N + 5/2)} \sum_{k=0}^{\infty} (k + 1) \frac{\Gamma(k + N + 5/2)}{\Gamma(k + N + 2)} t^{2k} \\
&= \frac{\Gamma(N + 2)}{\Gamma(N + 5/2)} t^{-2} \sum_{k=0}^{\infty} k \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 1)} t^{2k}, \\
{}_2F_1(1, N + 3/2, N + 1; t^2) &= \frac{\Gamma(N + 1)}{\Gamma(N + 3/2)} \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 1)} t^{2k}
\end{aligned}$$

and (3.9) we obtain that

$$\begin{aligned}
R(N, t) &= \left(3 + 4N - \frac{3t}{1-t}\right) \frac{\Gamma(N + 1)}{\Gamma(N + 3/2)} \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 1)} t^{2k} \\
&\quad + 4 \frac{N + 3/2}{N + 1} \frac{\Gamma(N + 2)}{\Gamma(N + 5/2)} \sum_{k=0}^{\infty} k \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 1)} t^{2k} \\
(3.19) \quad &= \frac{\Gamma(N + 1)}{\Gamma(N + 3/2)} \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 1)} \left(3 + 4N - \frac{3t}{1-t} + 4k\right) t^{2k}.
\end{aligned}$$

Let us consider the following series

$$S(N, t) := \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 1)} \left(3 + 4N - \frac{3t}{1-t} + 4k\right) t^{2k}.$$

We prove by induction with respect to N that $S(N, t) > 0$ for all $0 < t < 1$.

Let $N = 1$. Then from (3.18) and (3.19) by using (3.5) we get

$$\begin{aligned}
S(1, t) &= \frac{\Gamma(5/2)}{\Gamma(2)} R(1, t) = \frac{3\sqrt{\pi}}{4} \left(\frac{7 - 10t}{1-t} {}_2F_1(1, 5/2, 2; t^2) + 5t^2 {}_2F_1(2, 7/2, 3; t^2) \right) \\
&= \frac{3\sqrt{\pi}}{4} \left(\frac{7 - 10t}{1-t} {}_2F_1(1, 5/2, 2; t^2) + \frac{5t^2}{(1-t^2)^{5/2}} {}_2F_1(1, -1/2, 3; t^2) \right).
\end{aligned}$$

By using (3.6) we continue

$$\begin{aligned}
S(1, t) &= \frac{3\sqrt{\pi}}{4} \left(\frac{7 - 10t}{1-t} \frac{2(1 - (1-t^2)\sqrt{1-t^2})}{3t^2(1-t^2)\sqrt{1-t^2}} + 5t^2 \frac{4(-2 + 5t^2 + 2(1-t^2)^2\sqrt{1-t^2})}{15t^4(1-t^2)^{5/2}} \right) \\
&= \frac{3\sqrt{\pi} \left((2t + 3)t^2\sqrt{1-t^2} + 1 - \sqrt{1-t^2} \right)}{2(1-t)t^2(1+t)^2\sqrt{1-t^2}}.
\end{aligned}$$

Since $(2t + 3)t^2\sqrt{1-t^2} + 1 > 1$ and $\sqrt{1-t^2} < 1$ for $0 < t < 1$ we have that $(2t + 3)t^2\sqrt{1-t^2} + 1 - \sqrt{1-t^2} > 0$ and consequently $S(1, t) > 0$, $0 < t < 1$.

Further we assume that for $N \in \mathbb{N}$ the sum $S(N, t)$ is positive and we prove that $S(N + 1, t)$ is also positive. From (3.9) and the definition of the Gamma function we have

$$\begin{aligned} S(N + 1, t) &= \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 5/2)}{\Gamma(k + N + 2)} \left(3 + 4(N + 1) - \frac{3t}{1-t} + 4k \right) t^{2k} \\ &= \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 3/2) (k + N + 3/2)}{\Gamma(k + N + 1) (k + N + 1)} \left(3 + 4(N + 1) - \frac{3t}{1-t} + 4k \right) t^{2k}. \end{aligned}$$

By using simple transformations we proceed as follows

$$\begin{aligned} S(N + 1, t) &= \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 1)} \left(1 + \frac{1}{2k + 2N + 2} \right) \left(7 + 4N - \frac{3t}{1-t} + 4k \right) t^{2k} \\ &= \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 1)} \left(3 + 4N - \frac{3t}{1-t} + 4k \right) t^{2k} \\ &\quad + \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 1)} \left(6 + \frac{3}{2} \frac{1-2t}{k + N + 1} \right) t^{2k} \\ (3.20) \quad &= S(N, t) + \sigma(N, t), \end{aligned}$$

where

$$\sigma(N, t) := \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 1)} \left(6 + \frac{3}{2} \frac{1-2t}{k + N + 1} \right) t^{2k}.$$

For $0 < t \leq 1/2$ it is obvious that $\sigma(N, t) > 0$ for all $N \in \mathbb{N}$. Let now $1/2 < t < 1$. The sum $\sigma(N, t)$ can be rewritten in the following way

$$(3.21) \quad \sigma(N, t) = 6 \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 1)} t^{2k} - \frac{3(2t-1)}{2(1-t)} \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 2)} t^{2k}.$$

Let us further prove that $\sigma(N + 1, t) > \sigma(N, t)$, $N \in \mathbb{N}$. By $g(N)$ we denote $g(N) = \sigma(N + 1, t) - \sigma(N, t)$, $1/2 < t < 1$, and prove that $g(N) > 0$ for all $N \in \mathbb{N}$. We have

$$\begin{aligned} g(N) &= \sigma(N + 1, t) - \sigma(N, t) \\ &= 6 \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 1)} \left(\frac{k + N + 3/2}{k + N + 1} - 1 \right) t^{2k} \\ &\quad + \frac{3(2t-1)}{2(1-t)} \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 2)} \left(1 - \frac{k + N + 3/2}{k + N + 2} \right) t^{2k} \\ (3.22) \quad &= 6 \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 1)} \frac{1/2}{k + N + 1} t^{2k} \\ &\quad + \frac{3(2t-1)}{2(1-t)} \sum_{k=0}^{\infty} \frac{\Gamma(k + N + 3/2)}{\Gamma(k + N + 2)} \frac{1/2}{k + N + 2} t^{2k}. \end{aligned}$$

From (3.22) we see that $g(N) > 0$ for all $N \in \mathbb{N}$. Therefore, $\sigma(N, t) \geq \sigma(1, t)$ for all $N \in \mathbb{N}$. By using (3.4) and (3.21) we obtain

$$\sigma(1, t) = 6 \frac{\Gamma(5/2)}{\Gamma(2)} {}_2F_1(1, 5/2, 2; t^2) - \frac{3(2t-1)}{2(1-t)} \frac{\Gamma(5/2)}{\Gamma(3)} {}_2F_1(1, 5/2, 3; t^2).$$

By using (3.6) and simple transformations we have

$$(3.23) \quad \begin{aligned} \sigma(1, t) &= \frac{3\sqrt{\pi}(1 - (1 - t^2)\sqrt{1 - t^2})}{t^2(1 - t^2)\sqrt{1 - t^2}} - \frac{3\sqrt{\pi}(2t - 1)(2 - (2 + t^2)\sqrt{1 - t^2})}{4(1 - t)t^4\sqrt{1 - t^2}} \\ &= \frac{3\sqrt{\pi} \left(2 + (2t + t^3 + 6t^4)\sqrt{1 - t^2} - (2t + (2 + t^2)\sqrt{1 - t^2}) \right)}{4t^4(1 - t^2)^{3/2}}. \end{aligned}$$

Our further goal is to prove that for $1/2 < t < 1$

$$2 + (2t + t^3 + 6t^4)\sqrt{1 - t^2} > 2t + (2 + t^2)\sqrt{1 - t^2},$$

which follows from

$$2 - 2t > (2 - 2t + t^2 - t^3)\sqrt{1 - t^2} = (1 - t)(2 + t^2)\sqrt{1 - t^2},$$

that for $0 < t < 1$ is equivalent to $4 > 4 - 3t^4 - t^6$.

From this and (3.23) we have that $\sigma(1, t) > 0$ for $1/2 < t < 1$. Since $\sigma(N, t) > \sigma(1, t) > 0$ which together with the assumption $S(N, t) > 0$ and (3.20) implies $S(N + 1, t) > 0$. \square

4. APPROXIMATION OF THE FUNCTION $\exp(-B|\mathbf{x} - \mathbf{x}_0|^2)$ IN THE SPACE $L_2(\mathbb{R}^3, \omega_\lambda)$

In this section we prove formulas that show the behavior of SGL Fourier coefficients of Gaussian functions $w(\mathbf{x} - \mathbf{x}_0) = \exp(-B|\mathbf{x} - \mathbf{x}_0|^2)$ in the space $L_2(\mathbb{R}^3, \omega_\lambda)$ and present numerical results with respect to the behaviour of the quantity $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ for these functions. We consider two cases in the spherical coordinates: I. $\mathbf{x}_0 = (r_0, 0, 0)$; II. $\mathbf{x}_0 = (r_0, \theta_0, \varphi_0)$.

Further we use the following notations: let

$$p_{\lambda, r_0} := \frac{2B\sqrt{\lambda}r_0}{\sqrt{2B\lambda + 2}}, \quad C_{nl}^\lambda := \left(\frac{2\pi^2\lambda^{3/2}(2l+1)(n-l-1)!}{\Gamma(n+1/2)} \right)^{1/2},$$

and by $\Phi_{l,j,i}(t)$, $t \geq 0$, we denote

$$\begin{aligned} \Phi_{l,j,i}(t) &:= \frac{1}{(l-2i+1)\Gamma(\frac{l+2j+4}{2})} {}_2F_2 \left(\frac{l-2i+1}{2}, \frac{l+2j+3}{2}; \frac{1}{2}, \frac{l-2i+3}{2}; \frac{t^2}{2} \right) \\ &\quad - \frac{\sqrt{2}t}{(l-2i+2)\Gamma(\frac{l+2j+3}{2})} {}_2F_2 \left(\frac{l-2i+2}{2}, \frac{l+2j+4}{2}; \frac{3}{2}, \frac{l-2i+4}{2}; \frac{t^2}{2} \right), \end{aligned}$$

where ${}_2F_2$ is generalized hypergeometric function [7, 9.14] defined by

$${}_2F_2(a_1, a_2; b_1, b_2; t) = \sum_{k=0}^{\infty} \frac{(a_1)_k (a_2)_k z^k}{(b_1)_k (b_2)_k k!}.$$

I. Let at first $\mathbf{x}_0 = (r_0, 0, 0)$.

Theorem 4.1. *For the function $w(\mathbf{x} - \mathbf{x}_0) = \exp(-B|\mathbf{x} - \mathbf{x}_0|^2)$, $\mathbf{x}, \mathbf{x}_0 \in \mathbb{R}^3$, $\mathbf{x}_0 = (r_0, 0, 0)$, $B > 0$, and $\lambda > 0$ we have*

$$(4.1) \quad \begin{aligned} \widehat{w}_{nl0}^\lambda &= \exp(-Br_0^2) C_{nl}^\lambda \sum_{j=0}^{n-l-1} \frac{(-1)^j}{j!} \binom{n-1/2}{n-l-1-j} (4B\lambda + 4)^{-\frac{l+2j+3}{2}} \\ &\quad \times \Gamma(l+2j+3) \sum_{i=0}^{\lfloor l/2 \rfloor} \frac{(-1)^{l-i} (2l-2i)! (1 + (-1)^{l-2i})}{2^l i! (l-i)! (l-2i)!} \times \Phi_{l,j,i}(p_{\lambda, r_0}) \end{aligned}$$

and $\widehat{w}_{nlm}^\lambda = 0$, if $m \neq 0$.

Proof. The function $w(\mathbf{x} - \mathbf{x}_0) = \exp(-B|\mathbf{x} - \mathbf{x}_0|^2)$ can be rewritten in the spherical coordinates $\mathbf{x} = (r, \theta, \varphi)$ in the following way

$$w(r, \theta) = \exp(-B(r_0^2 + r^2 - 2rr_0 \cos \theta)).$$

Since $\overline{Y_{l,m}(\theta, \varphi)} = (-1)^m Y_{l,-m}(\theta, \varphi)$ we have

$$\begin{aligned} \widehat{w}_{nlm}^\lambda &= \int_0^\pi \int_0^{2\pi} \int_0^\infty w(r, \theta) \overline{H_{nlm}^\lambda(r, \theta, \varphi)} \exp(-r^2/\lambda) r^2 \sin \theta \, dr \, d\varphi \, d\theta \\ &= \left(\frac{2(n-l-1)!}{\lambda^{3/2} \Gamma(n+1/2)} \right)^{1/2} \left(\frac{(2l+1)(l+m)!}{4\pi(l-m)!} \right)^{1/2} (-1)^m \int_0^{2\pi} \exp(-im\varphi) \, d\varphi \\ (4.2) \quad &\times \int_0^\pi \int_0^\infty w(r, \theta) \exp(-r^2/\lambda) \left(r/\sqrt{\lambda} \right)^l L_{n-l-1}^{l+1/2}(r^2/\lambda) P_{l,-m}(\cos \theta) r^2 \sin \theta \, dr \, d\theta. \end{aligned}$$

Taking into account that

$$\int_0^{2\pi} \exp(-im\varphi) \, d\varphi = 2\pi \delta_{m0},$$

we get $\widehat{w}_{nlm}^\lambda = 0$ if $m \neq 0$.

Let now $m = 0$. For simplicity we denote

$$w_{nl}^\lambda := \exp(Br_0^2) \left(\frac{2\pi \lambda^{3/2} (n-l-1)! (2l+1)}{\Gamma(n+1/2)} \right)^{-1/2} \widehat{w}_{nl0}^\lambda.$$

Making change of variables $r/\sqrt{\lambda} \rightarrow t$ in (4.2), we obtain

$$w_{nl}^\lambda = \int_0^\pi \int_0^\infty \exp\left(2B\sqrt{\lambda}tr_0 \cos \theta\right) \exp(-(B\lambda+1)t^2) t^l L_{n-l-1}^{l+1/2}(t^2) P_l(\cos \theta) t^2 \sin \theta \, dt \, d\theta.$$

Using the closed form for associated Laguerre polynomials [7, 8.970 (1)]

$$L_n^\alpha(x) = \sum_{j=0}^n (-1)^j \binom{n+\alpha}{n-j} \frac{x^j}{j!},$$

we get

$$\begin{aligned} w_{nl}^\lambda &= \sum_{j=0}^{n-l-1} \frac{(-1)^j}{j!} \binom{n-1/2}{n-l-1-j} \\ &\times \int_0^\pi \int_0^\infty t^{(l+2j+3)-1} \exp\left(2B\sqrt{\lambda}tr_0 \cos \theta\right) \exp(-(B\lambda+1)t^2) P_l(\cos \theta) \sin \theta \, dt \, d\theta. \end{aligned}$$

From the formula [7, 3.462 (1)] for $\beta, \nu > 0$

$$\int_0^\infty x^{\nu-1} \exp(-\beta x^2 - \gamma x) \, dx = (2\beta)^{-\nu/2} \Gamma(\nu) \exp\left(\frac{\gamma^2}{8\beta}\right) D_{-\nu}\left(\frac{\gamma}{\sqrt{2\beta}}\right),$$

where D is the parabolic cylinder function (see [7, 9.24-9.25]), we have

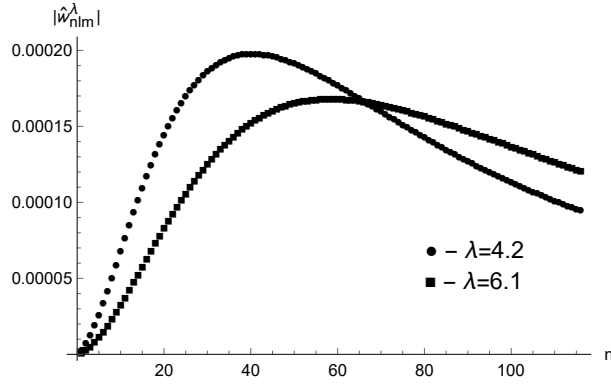


FIGURE 2. Plot of the behaviour of $|\widehat{w}_{nlm}^\lambda|$ ($B = 2$, $r_0 = 1$, $\theta_0 = \frac{\pi}{6}$, $\varphi_0 = \frac{\pi}{3}$) with respect to n ($l = 4$, $m = 3$).

$$(4.3) \quad w_{nl}^\lambda = \sum_{j=0}^{n-l-1} \frac{(-1)^j}{j!} \binom{n-1/2}{n-l-1-j} (2B\lambda+2)^{-\frac{l+2j+3}{2}} \Gamma(l+2j+3) \\ \times \int_0^\pi \exp\left(\frac{1}{4} p_{\lambda,r_0}^2 \cos^2 \theta\right) D_{-l-2j-3}(-p_{\lambda,r_0} \cos \theta) P_l(\cos \theta) \sin \theta \, d\theta,$$

where $p_{\lambda,r_0} = \frac{2B\sqrt{\lambda}r_0}{\sqrt{2B\lambda+2}}$.

Let us denote

$$(4.4) \quad I := \int_0^\pi \exp\left(\frac{1}{4} p_{\lambda,r_0}^2 \cos^2 \theta\right) D_{-l-2j-3}(-p_{\lambda,r_0} \cos \theta) P_l(\cos \theta) \sin \theta \, d\theta \\ = \int_{-1}^1 \exp\left(\frac{1}{4} p_{\lambda,r_0}^2 t^2\right) D_{-l-2j-3}(-p_{\lambda,r_0} t) P_l(t) \, dt.$$

By using the monomial representation of the Legendre polynomial [7, 8.911 (1)]

$$P_l(t) = \sum_{i=0}^{\lfloor l/2 \rfloor} (-1)^i \frac{(2l-2i)!}{2^l i! (l-i)! (l-2i)!} t^{l-2i},$$

we have

$$I = \sum_{i=0}^{\lfloor l/2 \rfloor} (-1)^i \frac{(2l-2i)!}{2^l i! (l-i)! (l-2i)!} \int_{-1}^1 \exp\left(\frac{1}{4} p_{\lambda,r_0}^2 t^2\right) D_{-l-2j-3}(-p_{\lambda,r_0} t) t^{l-2i} \, dt.$$

Making change of variables $-p_{\lambda,r_0} t \rightarrow y$ we obtain

$$I = \sum_{i=0}^{\lfloor l/2 \rfloor} \frac{(-1)^{i+1} (2l-2i)!}{2^l i! (l-i)! (l-2i)!} \left(-\frac{1}{p_{\lambda,r_0}}\right)^{l-2i+1} \int_{-p_{\lambda,r_0}}^{p_{\lambda,r_0}} y^{l-2i} \exp(y^2/4) D_{-l-2j-3}(y) \, dy.$$

From the formula [1]

$$\begin{aligned} \int z^{\mu-1} \exp(z^2/4) D_\nu(z) dz &= \frac{\sqrt{\pi} 2^{\nu/2} z^\mu}{\mu \Gamma(\frac{1-\nu}{2})} {}_2F_2\left(\frac{\mu}{2}, -\frac{\nu}{2}; \frac{1}{2}, \frac{\mu}{2} + 1; \frac{z^2}{2}\right) \\ &\quad - \frac{\sqrt{\pi} 2^{(\nu+1)/2} z^{\mu+1}}{(\mu+1) \Gamma(\frac{-\nu}{2})} {}_2F_2\left(\frac{\mu+1}{2}, \frac{1-\nu}{2}; \frac{3}{2}, \frac{\mu+3}{2}; \frac{z^2}{2}\right) \end{aligned}$$

we get

$$(4.5) \quad I = \sqrt{\pi} \sum_{i=0}^{\lfloor l/2 \rfloor} (-1)^{l-i} \frac{(2l-2i)!(1+(-1)^{l-2i})}{2^l i!(l-i)!(l-2i)!} 2^{-\frac{l+2j+3}{2}} \times \Phi_{l,j,i}(p_{\lambda,r_0}).$$

The relations (4.3), (4.4) and (4.5), taking into account the definition of w_{nl}^λ , imply (4.1). \square

II. Here we discuss the general case $\mathbf{x}_0 = (r_0, \theta_0, \varphi_0)$. Before formulating our next results let us first describe the main ideas of the rotational invariance property of spherical harmonics. We consider the expansion of a function $f \in L_2(\mathbb{R}^3, \omega_\lambda)$ in the SGL Fourier series. Taking into account the definition of the set Δ_n we obtain

$$f(r, \theta, \varphi) = \sum_{n=1}^{\infty} \sum_{l=0}^{n-1} \sum_{m=-l}^l \widehat{f}_{nlm}^\lambda H_{nlm}^\lambda(r, \theta, \varphi) = \sum_{n=1}^{\infty} \sum_{l=0}^{n-1} \sum_{m=-l}^l \widehat{f}_{nlm}^\lambda N_{nlm}^\lambda R_{nl}^\lambda(r) Y_{lm}(\theta, \varphi),$$

where the convergence is understood in the sense of the space $L_2(\mathbb{R}^3, \omega_\lambda)$.

Applying to the function f the Euler rotation operator $\widehat{R}(\alpha, \beta, \gamma)$, $\alpha, \gamma \in [0, 2\pi]$ and $\beta \in [0, \pi]$, we get (see, for example, [15, p. 37–44] for details)

$$\begin{aligned} \widehat{R}(\alpha, \beta, \gamma) f(r, \theta, \varphi) &= \sum_{n=1}^{\infty} \sum_{l=0}^{n-1} \sum_{m=-l}^l \widehat{f}_{nlm}^\lambda N_{nlm}^\lambda R_{nl}^\lambda(r) \widehat{R}(\alpha, \beta, \gamma) Y_{lm}(\theta, \varphi) \\ &= \sum_{n=1}^{\infty} \sum_{l=0}^{n-1} \sum_{m=-l}^l \widehat{f}_{nlm}^\lambda N_{nlm}^\lambda R_{nl}^\lambda(r) \sum_{m'=-l}^l Y_{lm'}(\theta, \varphi) \mathbf{D}_{m'm}^{(l)}(\alpha, \beta, \gamma) \\ &= \sum_{n=1}^{\infty} \sum_{l=0}^{n-1} \sum_{m'=-l}^l \left(\sum_{m=-l}^l \mathbf{D}_{m'm}^{(l)}(\alpha, \beta, \gamma) \widehat{f}_{nlm}^\lambda \right) N_{nlm'}^\lambda R_{nl}^\lambda(r) Y_{lm'}(\theta, \varphi), \end{aligned}$$

where $\mathbf{D}_{m'm}^{(l)}$ are the Wigner rotation matrices defined as follows

$$\mathbf{D}_{m'm}^{(l)}(\alpha, \beta, \gamma) = \exp(-im'\alpha) d_{m'm}^{(l)}(\beta) \exp(-im\gamma)$$

and

$$\begin{aligned} d_{m'm}^{(l)}(\beta) &= ((l+m')!(l-m')!(l+m)!(l-m)!)^{1/2} \\ &\quad \times \sum_{k=\max\{0, m-m'\}}^{\min\{l-m', l+m\}} \frac{(-1)^{k+m'-m} (\cos(\beta/2))^{2l+m-m'-2k} (\sin(\beta/2))^{2k+m'-m}}{(l+m-k)! k! (m'-m+k)! (l-m'-k)!}. \end{aligned}$$

In other words, if $\widehat{f}_{nlm}^\lambda$ are the SGL Fourier coefficients of a function f , the SGL Fourier coefficients of the function $g = \widehat{R}(\alpha, \beta, \gamma)f$ can be found by the formula

$$(4.6) \quad \widehat{g}_{nlm}^\lambda = \sum_{m'=-l}^l \mathbf{D}_{mm'}^{(l)}(\alpha, \beta, \gamma) \widehat{f}_{nlm'}^\lambda.$$

Finally, using the relation (4.6) and Theorem 4.1 we obtain formulas for the SGL Fourier coefficients of the function $w(\mathbf{x} - \mathbf{x}_0) = \exp(-B|\mathbf{x} - \mathbf{x}_0|^2)$, where in the spherical coordinates $\mathbf{x}_0 = (r_0, \theta_0, \varphi_0)$, and

$$w(r, \theta, \varphi) = \exp(-Br_0^2 - Br^2 + 2Brr_0(\sin \theta \sin \theta_0 \cos(\varphi - \varphi_0) + \cos \theta \cos \theta_0)).$$

Corollary 4.1. *For the function $w(\mathbf{x} - \mathbf{x}_0) = \exp(-B|\mathbf{x} - \mathbf{x}_0|^2)$, $B > 0$, $\mathbf{x}, \mathbf{x}_0 \in \mathbb{R}^3$, $\mathbf{x}_0 = (r_0, \theta_0, \varphi_0)$ and $\lambda > 0$ the following formula hold*

$$(4.7) \quad \widehat{w}_{nlm}^\lambda = \mathbf{D}_{m0}^{(l)}(\varphi_0, \theta_0, 0) \widehat{w}_{nl0}^\lambda,$$

where $\widehat{w}_{nl0}^\lambda$ is defined by (4.1).

The behavior of $|\widehat{w}_{nlm}^\lambda|$ with respect to indices n , l and m with fixed values of the other indices is presented in Figures 2 and 3.

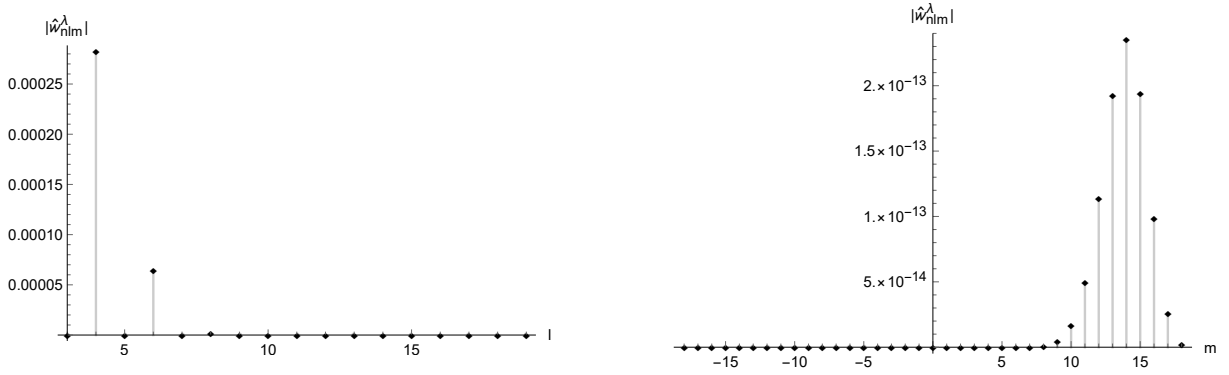


FIGURE 3. Plots of the behavior of $|\widehat{w}_{nlm}^\lambda|$ ($B = 2$, $r_0 = 1$, $\theta_0 = \frac{\pi}{6}$, $\varphi_0 = \frac{\pi}{3}$) with respect to l (left, $n = 20$, $m = 3$, $\lambda = 1$) and with respect to m (right, $n = 20$, $l = 18$, $\lambda = 1$).

For the case when $\mathbf{x}_0 \neq (0, 0, 0)$ it seems to be impossible to write results similar to Theorems 3.2, 3.3 and 3.4 due to the complex analytic representation of SGL Fourier coefficients of Gaussians (see Theorem 4.1 and Corollary 4.1). Therefore, in this case we use a computational method to investigate the behaviour of the quantity $\mathcal{E}_N(w, \mathcal{H}^\lambda)$. Let us further describe the main ideas of this method.

From the Parseval's equality we have

$$\begin{aligned} \mathcal{E}_N(w, \mathcal{H}^\lambda) &= \left\| w - \sum_{n=1}^N \left(\sum_{(l,m) \in \Delta_n} \widehat{w}_{nlm}^\lambda H_{nlm}^\lambda \right) \right\|_{L_2(\mathbb{R}^3, \omega_\lambda)} \\ &= \left(\sum_{n=N+1}^{\infty} \left(\sum_{(l,m) \in \Delta_n} |\widehat{w}_{nlm}^\lambda|^2 \right) \right)^{1/2}. \end{aligned}$$

Let us choose $N_0 \in \mathbb{N}$ from the condition

$$\sum_{(l,m) \in \Delta_n} |\widehat{w}_{nlm}^\lambda|^2 < \varepsilon \text{ for } n > N_0,$$

where ε is a very small positive number. Then we can assume that

$$(4.8) \quad \mathcal{E}_N(w, \mathcal{H}^\lambda) \approx \left(\sum_{n=N+1}^{N_0} \left(\sum_{(l,m) \in \Delta_n} |\widehat{w}_{nlm}^\lambda|^2 \right) \right)^{1/2}.$$

By using (4.8) and formulas for the SGL Fourier coefficients $\widehat{w}_{nlm}^\lambda$ from the Corollary 4.1 we can numerically compute approximate values of $\mathcal{E}_N(w, \mathcal{H}^\lambda)$. Analyzing numerical data we can conclude that in the case when $w(\mathbf{x} - \mathbf{x}_0) = \exp(-B|\mathbf{x} - \mathbf{x}_0|^2)$ and $\mathbf{x}_0 \neq 0$ the quantity $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ keeps its behaviour with respect to the parameter λ (compare Figure 1 (right) and Figure 4 (right)).

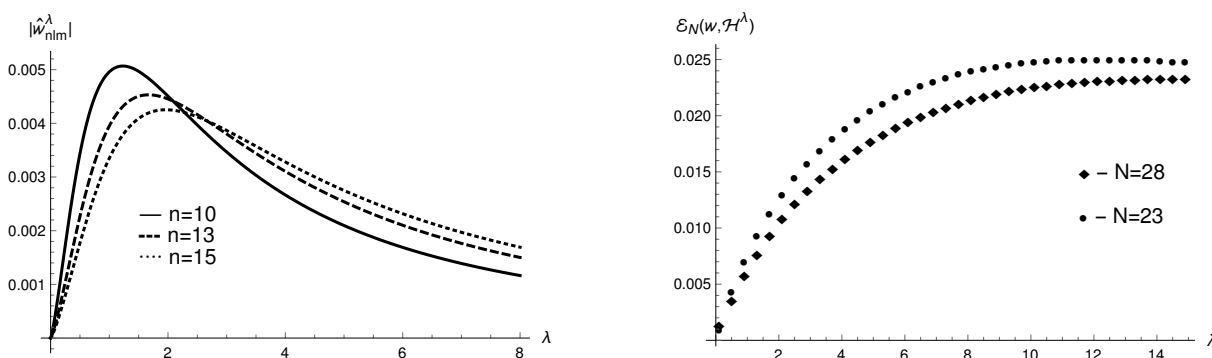


FIGURE 4. Plots of the behavior of $|\widehat{w}_{nlm}^\lambda|$ (left, $B = 2$, $\mathbf{x}_0 = (1, 0, 0)$ in the spherical coordinates, $l = 2$, $m = 0$) and $\mathcal{E}_N(w, \mathcal{H}^\lambda)$ (right, $B = 2$ and $\mathbf{x}_0 = (1, 0, 0)$ in the spherical coordinates) with respect to λ .

5. DISCUSSION, CONCLUSIONS AND POSSIBLE APPLICATIONS

In this section we describe one possible application of obtained results to the problem of molecular docking. Let us start with some known facts.

Gaussian functions are often used for approximation of the electron density distribution of molecules ([8], [9]). For example, for the atom k we have

$$\mathcal{K}(\mathbf{x} - \mathbf{x}_{ck}) = \exp\left(\frac{B|\mathbf{x} - \mathbf{x}_k|^2}{r_k^2} - B\right),$$

where $B < 0$ is the rate of decay parameter, r_k is the Van der Waals radius of the k th atom and $|\mathbf{x} - \mathbf{x}_k|^2 = (x - x_k)^2 + (y - y_k)^2 + (z - z_k)^2$, where $\mathbf{x}_k = (x_k, y_k, z_k)$ is the center of the k th atom. A volumetric representation of the molecule may now be obtained by summing the contributions from each single atom, i.e. the electron density for a molecule with M atoms is described as

$$\sum_{k=1}^M \mathcal{K}(\mathbf{x} - \mathbf{x}_k) = \sum_{k=1}^M \exp\left(\frac{B|\mathbf{x} - \mathbf{x}_k|^2}{r_k^2} - B\right).$$

To choose a suitable scoring function is the crucial part in all docking approaches. Some papers (see, for instance, [11]) consider the approach of separation the affinity functions into

core and skin regions with further goal to penalize core-core clashes and add positive skin–skin overlaps. Using positive real values as the weights for the smooth particle representation of the affinity function defined over the skin and imaginary values in the representation of the core regions, yields negative numbers for core-core overlaps and positive numbers for skin-skin overlaps during the convolution. So, the weighted affinity function for the molecule \mathbf{A} takes the form

$$Q^{\mathbf{A}}(\mathbf{x}) = \sum_{k=1}^M \gamma_k^{\mathbf{A}} \mathcal{K}(\mathbf{x} - \mathbf{x}_k),$$

where

$$\gamma_k^{\mathbf{A}} = \begin{cases} 1, & \mathbf{x}_k \in \text{Skin } \mathbf{A}, \\ \rho i, & \mathbf{x}_k \in \text{Core } \mathbf{A}, \end{cases}$$

and $\rho \gg 1$.

Let $\widehat{R}(\alpha, \beta, \gamma)$ and $\widehat{R}'(0, \beta', \gamma')$ be the Euler rotation operators (see Section 4 and [15, p. 37–44]). The notation $Q_{\widehat{R}}^{\mathbf{A}}$ means that we apply the operator \widehat{R} to the function $Q^{\mathbf{A}}$. By $T^{\boldsymbol{\tau}}$ we denote the operator of the shift on the vector $\boldsymbol{\tau} = (\tau, 0, 0)$, i.e. $T^{\boldsymbol{\tau}}Q^{\mathbf{A}}(\mathbf{x}) = Q^{\mathbf{A}}(\mathbf{x} - \boldsymbol{\tau})$. We consider the search algorithm suggested by Ritchie [15, Chapter 4]. The main ideas of this algorithm is to use the Fast Rotational Matching approach, i.e. consideration of the rigid docking with the $6D$ search space $(\alpha, \beta, \gamma, \beta', \gamma', \tau)$.

The convolution search scoring is defined by

$$(5.1) \quad C(\widehat{R}, \widehat{R}', \mathbf{t}) = \text{Re} \left(\int_{\mathbb{R}^3} Q_{\widehat{R}}^{\mathbf{A}}(\mathbf{x}) T^{\boldsymbol{\tau}} Q_{\widehat{R}'}^{\mathbf{B}}(\mathbf{x}) \omega_{\lambda}(\mathbf{x}) d\mathbf{x} \right)$$

and the solution of the docking problem is the pair $(\widehat{R}_{\max}, \widehat{R}'_{\max}, \boldsymbol{\tau}_{\max})$ for which

$$C(\widehat{R}_{\max}, \widehat{R}'_{\max}, \boldsymbol{\tau}_{\max}) = \max_{(\widehat{R}, \widehat{R}', \boldsymbol{\tau})} C(\widehat{R}, \widehat{R}', \boldsymbol{\tau}).$$

By using expansions of the corresponding scoring functions in the SGL Fourier series we get

$$C(\widehat{R}, \widehat{R}', \boldsymbol{\tau}) \approx \text{Re} \left(\sum_{nlm}^N \sum_{n'l'm'}^N \int_{\mathbb{R}^3} \widehat{(Q_{\widehat{R}}^{\mathbf{A}})}_{nlm}^{\lambda} \widehat{(T^{\boldsymbol{\tau}} Q_{\widehat{R}'}^{\mathbf{B}})}_{nlm}^{\lambda} H_{nlm}^{\lambda}(\mathbf{x}) H_{n'l'm'}^{\lambda}(\mathbf{x}) \omega_{\lambda}(\mathbf{x}) d\mathbf{x} \right).$$

The docking integral (5.1) depends on the scale factor λ . For the optimization of the computations of scoring for given molecules \mathbf{A} and \mathbf{B} one should use a suitable value of the parameter λ . In [15, p. 34] it is shown that with an order of expansion $N = 28$ the SGL basis functions give good level of recovery of molecular shape. We translate and scale the docking region to the unit ball and are oriented on the most distant atom. Then one can choose values of λ based on Figure 4 (right). However, the values really close to zero can not be used since then the weighed Gaussian function together with basis functions tends to zero and the basis elements can not provide good sampling for the recovery of the molecular shape. On the other hand, using small λ in naive computations can cause computational inaccuracy.

Acknowledgements. The authors were supported by H2020-MSCA-RISE-2014 Project number 645672 (AMMODIT: Approximation Methods for Molecular Modelling and Diagnosis Tools). The authors would like to thank Viktor Romanyuk (Institute of Mathematics NAS Ukraine) for valuable remarks regarding this paper.

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