Applied Mathematics & Information Sciences
An International Journal

http://dx.doi.org/10.12785/amis/090634

Fourier Transform of Bessel Type Functions

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Received: 2 Mar. 2015, Revised: 30 Apr. 2015, Accepted: 1 May 2015
Published online: 1 Nov. 2015

Abstract: Bessel type functions (BTFs), which are one of the types of exponential type functions (ETFs), are used usually as basis functions in the multi-center atomic and molecular integrals to better understand physical and chemical properties of matter. As a general rule, the most promising approach for the calculation of multi-center integrals appears to be the called the Fourier transform method (FTM) where multi-center integrals are transformed into inverse Fourier integrals. In this approach, basis functions have not simplicity to make mathematical operations, but their Fourier transforms are easier to use. In this work, with the help of FTM and some properties of Bessel functions, we present new mathematical results for the Fourier transform of normalized BTFs in terms of Gegenbauer polynomials and hypergeometric functions. Moreover, we compare mathematical results for new equations in a table and other details of evaluation method are discussed.

Keywords: Bessel type functions, Fourier transform, Gegenbauer polynomials, Hypergeometric functions

1 Introduction

Recently, there is an important interest to the some types of bessel functions and their mathematical applications that are most frequently used in solving various problems arising in natural sciences (mathematics, physics, mechanics, astronomy, engineering, etc.). Some of these recent researches can be given in the references: [1,2,3,4]. BTFs are one of the types of ETFs which are first introduced by Filter and Steinborn [5]. In the solution of molecular integrals, multi-center molecular integrals have to be computed in *ab initio* quantum chemical linear combination of atomic orbitals (LCAO) and multi-center calculations. It is advantageous to use a basis set of BTFs have properties of ETFs and, hence, allow to describe correctly the nuclear cusps and the large-distance behavior of the atomic wavefunctions [6]. In this work, we will focuse on the BTFs which are containing bessel functions actually. In the studies of mathematical, atomic and molecular physics with help of approximation methods, a suitable basis function must be selected. A good basis function for molecular calculations should satisfy two basic requirements [7]: first, short expansions of the atomic in the terms of the basis functions yield a good accuracy and second, the molecular multi-center integrals which occur inevitably and in very large quantum numbers in that approach can be computed efficiently. Among the ETFs, Slater type functions (STFs), which were introduced by Slater in his article on shielding constants [8], have the simplest analytical structure of all exponentially decreasing functions. Other commonly occurring functions of that class, for instance, hydrogen eigenfunctions, can normally be expressed quite easily as linear combinations of STFs. This implies that multi-center integrals of other exponentially decreasing functions can be expressed in terms of the basic multi-center integrals over STFs [9,10,11].

Currently, the most promising approach for the evaluation of molecular integrals appears to be the so called Fourier transform method where multi-center integrals are transformed into inverse Fourier integrals [12,13,14]. In this approach, it is not the analytical simplicity of basis function that matters but the analytical simplicity of its Fourier transform. In case of using analytical expressions of STFs is not giving a simplicity in calculations, but Fourier transform of STFs are very useful for evaluation of multi-center molecular integrals, especially for overlap integrals. Overlap integrals are also an important intermediate step for the derivation of all other multi-center integrals. The evaluation of overlap and other multi-center integrals over STFs is already today the bottleneck of any *ab initio* calculation in terms of accurate functions which have to satisfy the requirements of cusp condition and exponential decay. This explains the continued effort of theoretical investigation in this

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field, from the early study of Roothaan and Ruedenberg [15,16,17], Coulson [18], Löwdin [19], up to more recent work by Silverstone [20], Steinborn [5], Jones [21], Rinaldi's groups [22].

If we compare the structures of the Fourier transforms of STFs and BTFs it seems safe to conclude that overlap integrals of BTFs will be more compact and better suited for numerical applications than the corresponding integrals of STFs. Thus, BTFs are very simple ETFs in momentum space, in contrast to STFs which have relatively complicated Fourier transforms and which are only simple in coordinate space [7]. The Fourier transforms of other exponentially decreasing functions such as STFs or hydrogen eigenfunctions are significantly more complicated. In papers by Niukkanen [23], Weniger and Steinborn [7,24], and Weniger [25] it was shown that Fourier transforms of all commonly occurring exponentially decreasing functions can be expressed as linear combination of Fourier transforms of BTFs.

This paper is structured as follows. Section 2 provides general properties of BTFs and other necessary mathematical and physical relations. In Section 3, FTM has been explained and we describe the Fourier transforms of BTFs and STFs with their normalization coefficients. Besides, we obtain two new equations for Fourier transforms of normalized BTFs in terms of Gegenbauer polynomials and hypergeometric functions. Finally, in section 4, some numerical calculations in a table and a graph have been discussed to have a better understanding of aim of this work.

2 Definitions and Basic Relations

In this section, we first will define general properties for calculation which are needed later. The unnormalized real BTFs with the integer values of n, l, and m quantum numbers and α screening parameter [5]

$$B^m_{n,l}(\alpha,\mathbf{r}) = \left[2^{n+l}(n+l)!\right]^{-1} \hat{k}_{n-1/2}(\alpha r)\, S^m_l(\alpha\mathbf{r}) \quad (1)$$

is given by reduced Bessel functions [26,27]

$$\hat{k}_\nu(z) = (2/\pi)^{1/2} z^\nu K_\nu(z) \quad (2)$$

here, $K_\nu(z)$ are modified Bessel functions of the second kind [28]. For half-integral values of ν the reduced Bessel functions are polynomials in z multiplied by $\exp(-z)$ [27]. If the order ν assumes half-integral values, $\nu = n-1/2$, $n \in \mathbf{N}$, the reduced Bessel functions can be represented by an exponential multiplied by a polynomial [27]

$$\hat{k}_{n-1/2}(z) = e^{-z} \sum_{q=1}^{n} \frac{(2n-q-1)!}{(q-1)!\,(2n-2q)!!} z^{q-1} \quad (3)$$

In the half-integral orders, $\nu = n+1/2$, $n = 0, 1, \ldots$, the reduced Bessel functions can be represented as an exponential multiplied by a polynomial, which can also be written as a terminating confluent hypergeometric function [27]

$$\hat{k}_{n+1/2}(z) = e^{-z} \sum_{q=1}^{n} \frac{(2n-q)!}{q!\,(2n-2q)!!} z^q = (2n-1)!!\, e^{-z}\, {}_1F_1(-n;-2n;2z) \quad (4)$$

The angular part of the BTFs is given by regular solid harmonics [29]

$$S^m_l(\mathbf{r}) = r^l Y^m_l(\theta,\phi) \quad (5)$$

for the irregular solid harmonics

$$\pounds^m_l(\mathbf{r}) = r^{-l-1} Y^m_l(\theta,\phi) \quad (6)$$

Spherical harmonics $Y^m_l(\theta,\phi)$ can be real or complex [29]:

$$Y^m_l(\theta,\phi) = P_{l|m|}(\cos\theta)\, \Phi_m(\phi) \quad (7)$$

here $P_{l|m|}$ are normalized associated Legendre functions and for real spherical harmonics

$$\Phi_m(\phi) = \frac{1}{\sqrt{\pi(1+\delta_{m,0})}} \begin{cases} \cos(|m|\,\phi), & \text{for } m \geq 0 \\ \sin(|m|\,\phi), & \text{for } m < 0 \end{cases} \quad (8)$$

for complex spherical harmonics

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \quad (9)$$

For the integral of the product of three spherical harmonics over the surface of the unit sphere, so-called Gaunt coefficient [30];

$$\langle l_3 m_3 | l_2 m_2 | l_1 m_1 \rangle = \int \left[Y^{m_3}_{l_3}(\theta,\phi)\right]^* Y^{m_2}_{l_2}(\theta,\phi)\, Y^{m_1}_{l_1}(\theta,\phi)\, d\Omega \quad (10)$$

Gaunt coefficients are linearize the product of two spherical harmonics by defined following form:

$$\left[Y^{m_1}_{l_1}(\theta,\phi)\right]^* Y^{m_2}_{l_2}(\theta,\phi) = \sum_{l=l_{\min}}^{l_{\max}} {}^{(2)} \langle l_2\, m_2 | l_1\, m_1 | l\, m_2 - m_1 \rangle\, Y^{m_2-m_1}_l(\theta,\phi) \quad (11)$$

The symbol $\sum^{(2)}$ indicates that the summation proceeds in steps of 2. The summation limits in Eq. (11) determined by the selection rules satisfied by the Gaunt coefficients [31].

Normalized BTFs are [32]

$$\hat{B}^m_{n,l}(\alpha,\mathbf{r}) = \alpha^{3/2} N_{n,l} B^m_{n,l}(\alpha,\mathbf{r}) \quad (12)$$

$$N_{n,l} = \left(\frac{(2n+2l+1)!}{(1/2)_{2n+l}\,(1/2)_{l+1}}\right)^{1/2} \quad (13)$$

The unnormalized STFs which are defined by [5]

$$x_{n,l}^{m}(\alpha,\mathbf{r}) = (\alpha r)^{n-1}\exp(-\alpha r)\,Y_{l}^{m}(\theta,\varphi) \tag{14}$$

The normalized STFs are [33]

$$\hat{\chi}_{n,l}^{m}(\alpha,\mathbf{r}) = N_{n}(\alpha)\,\chi_{n,l}^{m}(\alpha,\mathbf{r}) \tag{15}$$

$$N_{n}(\alpha) = \alpha^{-n+1}\left[(2\alpha)^{2n+1}/(2n)!\right]^{1/2} \tag{16}$$

and also in Eq. (13), Pochhammer symbols [28]

$$(a)_{n} = \frac{\Gamma(a+n)}{\Gamma(a)} = \begin{cases} \prod_{j=1}^{n}(a+j-1) & \text{, for } n>0 \\ 1 & \text{, for } n=0 \end{cases} \tag{17}$$

There are some relations between STFs and BTFs. In other words, STF molecular integrals can be written as finite linear combinations of molecular integrals for BTFs, and vice versa. One of the these relations is [34]

$$\hat{\chi}_{l+1,l}^{m}(\alpha,\mathbf{r}) = \hat{B}_{1,l}^{m}(\alpha,\mathbf{r}) \tag{18}$$

STFs and BTFs can be written in terms of each other as [35]

$$\chi_{n,l}^{m}(\alpha,\mathbf{r}) = \sum_{\rho=\rho_{\min}}^{n-l}\frac{(-1)^{n-l-\rho}(n-l)!2^{l+\rho}(l+\rho)!}{(2\rho-n-l)!\,(2n-2l-2\rho)!!}B_{\rho,l}^{m}(\alpha,\mathbf{r}) \tag{19}$$

$$\rho_{\min} = \begin{cases} (n-l)/2, & \text{if } n-l \text{ is even} \\ (n-l+1)/2, & \text{if } n-l \text{ is odd} \end{cases} \tag{20}$$

$$B_{n,l}^{m}(\alpha,\mathbf{r}) = [(2n+2l)!!]^{-1}\sum_{\rho=1}^{n}\frac{(2n-\rho-1)!2^{\rho-n}}{(\rho-1)!\,(n-\rho)!}\chi_{\rho+l,l}^{m}(\alpha,\mathbf{r}) \tag{21}$$

3 Fourier Transform of Normalized BTFs

In this paper, we shall use the symmetric version of the Fourier transform, i.e., a given function $f(\mathbf{r})$ and its Fourier transform $F(\mathbf{p})$ are connected by the relationships

$$F(\mathbf{p}) = (2\pi)^{-3/2}\int e^{-i\mathbf{p}\cdot\mathbf{r}}f(\mathbf{r})\,d^{3}r \tag{22}$$

$$f(\mathbf{r}) = (2\pi)^{-3/2}\int e^{i\mathbf{p}\cdot\mathbf{r}}F(\mathbf{p})\,d^{3}p \tag{23}$$

In connection with multi-center integrals in general and with the spherical tensor gradient operator in special, the Fourier transform suffers from a serious limitation which must not be ignored. Classically, the Fourier transforms are defined only for functions that are absolutely integrable that belong to function space $L^{1}(R^{3})$, but by means of a suitable limiting procedure it can be extended uniquely to give a unitary map from the Hilbert space $L^{2}(R^{3})$ of square integrable functions onto itself [36].

The practical usefulness of FTM is obvious, and it would clearly beyond the scope of this study to mention all successful scientific applications. Let we just mention that Fourier transform is as first shown by Prosser and Blanchard [37] and by Geller [38] one of the principal methods of handling molecular multi-center integrals. The main advantage of the representation of two-center integrals as inverse Fourier integrals according to two-center integrals is that a separation of integration variables can be achieved quite easily if $f(\mathbf{r})$ and its Fourier transform $F(\mathbf{p})$are irreducible spherical tensors. With the help of FTM, according to

$$\iint f^{*}(\mathbf{r}_{1})\,g(\mathbf{r}_{2})\,h(\mathbf{r}_{1}-\mathbf{r}_{2})\,d^{3}r_{1}\,d^{3}r_{2} = (2\pi)^{3/2}\int \bar{f}^{*}(\mathbf{p})\,\bar{g}(\mathbf{p})\,\bar{h}(\mathbf{p})\,d^{3}p \tag{24}$$

Hence, with the help of the FTM, some six-dimensional integrals in configuration space with nonseparated integration variables can be transformed into three-dimensional integrals in momentum space where the integration variables can be separated quite easily if f, g, and h are irreducible spherical tensors.

For the evaluation of the Fourier transform of BTFs, we only have to express the well-known Rayleigh expansion of a plane wave in terms of spherical Bessel functions and spherical harmonics [39]

$$e^{\pm i\mathbf{x}.\mathbf{y}} = 4\pi\sum_{l=0}^{\infty}\sum_{m=-l}^{l}(\pm i)^{l}j_{l}(xy)\left[(Y_{l}^{m}(\theta_{x},\phi_{x}))^{*}Y_{l}^{m}(\theta_{y},\phi_{y})\right] \tag{25}$$

where

$$j_{l}(xy) = \left(\frac{\pi}{2xy}\right)^{1/2}J_{l+1/2}(xy) \tag{26}$$

is the spherical Bessel functions [40].

Fourier transform of unnormalized BTFs is [7]

$$B_{n,l}^{m}(\alpha,\mathbf{p}) = (2\pi)^{-3/2}\int e^{-i\mathbf{p}.\mathbf{r}}B_{n,l}^{m}(\alpha,\mathbf{r})\,d^{3}r \tag{27}$$

$$= (2\pi)^{1/2}\frac{\alpha^{2n+l-1}}{(\alpha^{2}+p^{2})^{n+l+1}}S_{l}^{m}(-i\mathbf{p}) \tag{28}$$

By taking Eqs. (12), (13), (27) and (28) into consideration, then Fourier transform of normalized BTFs can be denoted as

$$\hat{B}_{n,l}^{m}(\alpha,\mathbf{p}) = (2\pi)^{-3/2}\int e^{-i\mathbf{p}.\mathbf{r}}\hat{B}_{n,l}^{m}(\alpha,\mathbf{r})\,d^{3}r \tag{29}$$

$$= \alpha^{3/2}N_{n,l}(2\pi)^{-3/2}\int e^{-i\mathbf{p}.\mathbf{r}}B_{n,l}^{m}(\alpha,\mathbf{r})\,d^{3}r \tag{30}$$

$$= (2\pi)^{1/2}\left(\frac{(2n+2l+1)!}{(1/2)_{2n+l}(1/2)_{l+1}}\right)^{1/2}\frac{\alpha^{2n+l+1/2}}{(\alpha^{2}+p^{2})^{n+l+1}}S_{l}^{m}(-i\mathbf{p}) \tag{31}$$

The Fourier transform of normalized STFs are given by [41]

$$\hat{\chi}^m_{n,l}(\alpha,\mathbf{p}) = \frac{2^{n+l+1}\alpha^{n+1/2}l!(n-l)!}{\sqrt{\pi}(2n)!(\alpha^2+p^2)^{(n+l+2)/2}} C^{l+1}_{n-l}\left(\frac{\alpha}{\sqrt{\alpha^2+p^2}}\right) S^m_l(-i\mathbf{p}) \tag{32}$$

where, $C^{\alpha}_n(x)$ is the Gegenbauer polynomials as defined following form [40].

$$C^{\alpha}_n(x) = \sum_{s=0}^{E(n/2)} (-1)^s \frac{(\alpha+n-s-1)!}{(\alpha-1)!s!(n-2s)!}(2x)^{n-2s} \tag{33}$$

and

$$E(n/2) = \frac{n}{2} - \frac{1-(-1)^n}{4} \tag{34}$$

Now, let's find the Fourier transform of normalized BTFs in terms of Gegenbauer polynomials. First, with help of Eqs. (1), (3), (12) and (13), normalized BTFs can be written by linear combination of spherical harmonics as

$$\hat{B}^m_{n,l}(\alpha,\mathbf{r}) = \alpha^{3/2}\left(\frac{(2n+2l+1)!}{(1/2)_{2n+l}(1/2)_{l+1}}\right)^{1/2}\left[2^{n+l}(n+l)!\right]^{-1}\cdot e^{-\alpha r}\sum_{q=1}^{n}\frac{(2n-q-1)!}{(q-1)!(2n-2q)!!}(\alpha r)^{q+l-1}Y^m_l(\theta,\phi) \tag{35}$$

If we insert Eq. (35) into the Eq. (27), we can write

$$\hat{B}^m_{n,l}(\alpha,\mathbf{p}) = (2\pi)^{-3/2}\int e^{-i\mathbf{p}.\mathbf{r}}\hat{B}^m_{n,l}(\alpha,\mathbf{r})\,d^3r \tag{36}$$

$$= (2\pi)^{-3/2}\left(\frac{(2n+2l+1)!}{(1/2)_{2n+l}(1/2)_{l+1}}\right)^{1/2}\left[2^{n+l}(n+l)!\right]^{-1}\cdot \sum_{q=1}^{n}\frac{(2n-q-1)!}{(q-1)!(2n-2q)!!}\alpha^{l+q+1/2}\int e^{-i\mathbf{p}.\mathbf{r}}e^{-\alpha r}r^{q+l-1}Y^m_l(\theta,\phi)d^3r \tag{37}$$

Substituting Eq. (25) and Eq. (26) into the integral in Eq. (37) and using the orthogonality of the real spherical harmonics, then, Eq. (37) can be rewritten as

$$\hat{B}^m_{n,l}(\alpha,\mathbf{p}) = \left(\frac{(2n+2l+1)!}{(1/2)_{2n+l}(1/2)_{l+1}}\right)^{1/2}\left[2^{n+l}(n+l)!\right]^{-1}p^{-1/2}\cdot \sum_{q=1}^{n}\frac{(2n-q-1)!}{(q-1)!(2n-2q)!!}\alpha^{l+q+1/2}(-i)^l Y^m_l(\mathbf{p}/p)\cdot \int_0^{\infty} e^{-\alpha r}J_{l+1/2}(pr)r^{q+l+1/2}dr \tag{38}$$

For the solution of integral form in the Eq. (38), we will use the following relations separately [40]

$$\int_0^{\infty} e^{-\alpha r}J_{l+1/2}(pr)\,r^{k+1/2}dr = \frac{l!\,(k-l)!}{\sqrt{\pi}(\alpha^2+p^2)^{\frac{k+l+2}{2}}}(2p)^{(2l+1)/2}C^{l+1}_{k-l}\left(\frac{\alpha}{\sqrt{\alpha^2+p^2}}\right) \tag{39}$$

$$\int_0^{\infty} e^{-\alpha r}J_{\nu}(pr)\,r^{\mu-1}dr = \frac{\left(\frac{p}{2\alpha}\right)^{\nu}\Gamma(\nu+\mu)}{\alpha^{\mu}\Gamma(\nu+1)}\,{}_2F_1\left(\frac{\nu+\mu}{2},\frac{\nu+\mu+1}{2};\nu+1;-\frac{p^2}{\alpha^2}\right) \tag{40}$$

These integral representations can be used to solve our integral form in Eq. (38), and then with help of regular solid harmonics in Eq. (5), and with Eq. (39), for $k=q+l$, finally, the Fourier transform of normalized BTFs can be written in terms of Gegenbauer polynomials by

$$\hat{B}^m_{n,l}(\alpha,\mathbf{p}) = \left(\frac{(2n+2l+1)!}{(1/2)_{2n+l}(1/2)_{l+1}}\right)^{1/2}\left[2^{n+l}(n+l)!\right]^{-1}\cdot \sum_{q=1}^{n}\frac{(2n-q-1)!}{(q-1)!(2n-2q)!!}\alpha^{l+q+1/2}\cdot \frac{2^{l+1/2}l!q!}{\sqrt{\pi}(\alpha^2+p^2)^{(q+2l+2)/2}}C^{l+1}_q\left(\frac{\alpha}{\sqrt{\alpha^2+p^2}}\right)S^m_l(-i\mathbf{p}) \tag{41}$$

In the same way, by using integral form in Eq. (40), for $\nu = l+1/2$ and $\mu = q+l+3/2$, then, the Fourier transform of normalized BTFs can be obtained in terms of hypergeometric functions as follow

$$\hat{B}^m_{n,l}(\alpha,\mathbf{p}) = \left(\frac{(2n+2l+1)!}{(1/2)_{2n+l}(1/2)_{l+1}}\right)^{1/2}\left[2^{n+l}(n+l)!\right]^{-1}\cdot \sum_{q=1}^{n}\frac{(2n-q-1)!}{(q-1)!(2n-2q)!!}\frac{\alpha^{3l+2q+5/2}}{2^{l+1/2}}\frac{\Gamma(2l+q+2)}{\Gamma(l+3/2)}\cdot {}_2F_1\left(\frac{2l+q+2}{2},\frac{2l+q+3}{2};l+3/2;-\frac{p^2}{\alpha^2}\right)S^m_l(-i\mathbf{p}) \tag{42}$$

4 Summary and Conclusion

If Eqs. (41) and (42) are taken into consideration, in the two equations, angular parts $S^m_l(-i\mathbf{p})$ regular solid harmonics are the same. But, their radial parts are different. Fourier transform of BTFs in Eq. (41) has been obtained in terms of Gegenbauer polynomials, but in Eq. (42), it has been obtained in terms of hypergeometric functions. Although radial part of Eqs. (41) and (42) are different functions, we can see from Table 1 that their

Table 1: Comparison of numerical results for radial part of Fourier transform of normalized BTFs.

n	l	α	p	Radial part of Eq. (41)	Radial part of Eq. (42)
1	1	1	1	9.21318×10^{-1}	9.21318×10^{-1}
2	1	1	1	7.52253×10^{-1}	7.52253×10^{-1}
2	2	1	1	8.60694×10^{-1}	8.60694×10^{-1}
3	2	1	2	2.64782×10^{-3}	2.64782×10^{-3}
6	5	1	2	5.9318×10^{-6}	5.9318×10^{-6}
8	8	1	2	4.45546×10^{-8}	4.45546×10^{-8}
12	10	1	3	6.31312×10^{-18}	6.31312×10^{-18}
15	12	1	3	8.2872×10^{-22}	8.2872×10^{-22}

calculated numerical results are completely same. This situation proves that new obtained relations for Fourier transform of normalized BTFs are correct.

Normally, behaviors of graph of Gegenbauer polynomials and hypergeometric functions are not similar. When we take into account Figure 1, radial functions in Eqs. (41) and (42) generates same graphs even if they include Gegenbauer polynomials and hypergeometric functions. It can be seen from Figure 1 that graphs of radial part of Fourier transform of BTFs exponentially decrease. In other words, Fourier transform of BTFs are also one type of the other ETFs. Therefore, it can be easily said that our new analytical and computational findings are correct. The values of quantum numbers in the Table 1 and Figure 1 are used in the atomic units.

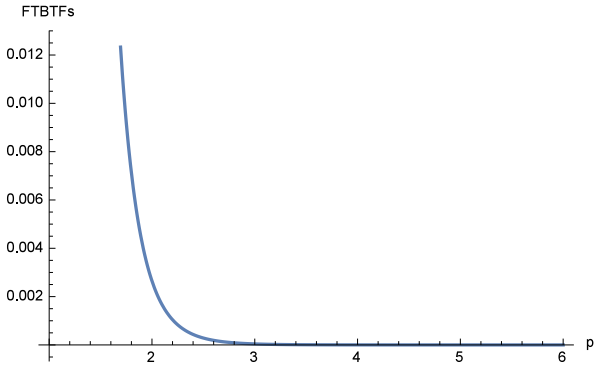

Fig. 1: Graph of radial part of Fourier transform of normalized BTFs (FTBTFs) versus p for quantum numbers $n = 3$, $l = 2$, and atomic screening parameter $\alpha = 1$. This graph can be ploted by using Eq. (41) or (42).

In this study we analyzed the analytical and numerical properties of Fourier transform of BTFs. We give new and useful mathematical relations for Fourier transform of BTFs, and they will contribute to the development of the other ETFs. Because, by using our method, new mathematical expressions and Fourier transforms can be derived for other molecular basis functions. Consequently, we would like to say that obtained equations in this paper for Fourier transform of normalized BTFs can be used in the future molecular integral calculations and mathematical applications.

References

[1] M. K. Kerimov, Comp. Math. Math. Phys., **54**, 9, 1387-1441 (2014).
[2] J. R. Kamm, T. O. Williams, J. S. Brock and S. Li, Int. J. Numer. Meth. Biomed. Engng., **26**, 1276-1292 (2010).
[3] V. A. Abilov and M. K. Kerimov, Comp. Math. Math. Phys., **52**, 6, 836-845 (2012).
[4] R. E. Gaunt, J. Math. Anal. Appl., **420**, 1, 373-386 (2014).
[5] E. Filter, E. O. Steinborn, Phys. Rev **A 18**, 1-11 (1978).
[6] H. H. H. Homeier, E. O. Steinborn, Comput. Phys. Commun., **77**, 135-151 (1993).
[7] E. J. Weniger, E. O. Steinborn, J. Chem. Phys., **78**, 6121-6132 (1983).
[8] J. C. Slater, Phys. Rev., **36**, 57-64 (1930).
[9] M. Yavuz, N. Yükçü, E. Öztekin, S. Döndür, and H. Yilmaz, Commun. Theor. Phys., **43**, 151-158 (2005).
[10] N. Yükçü, İ. Şenlik, E. Öztekin, Int. J. Quantum Chem., **112**, 2, 414-425 (2012).
[11] N. Yükçü, E. Öztekin, Adv. Quantum Chem., **67**, 9, 231-243 (2013).
[12] H. P. Trivedi, E. O. Steinborn, Phys. Rev. **A 27**, 670-679 (1983).
[13] J. Grotendorst, E O Steinborn, J. Comput. Phys., **61**, 195-217 (1985).
[14] E. J. Weniger, J. Grotendorst, E. O. Steinborn, Phys. Rev. **A 33**, 3688-3705 (1986).
[15] C. C. J Roothaan, J. Chem. Phys., **19**, 1445-1458 (1951).
[16] K. Ruedenberg, J. Chem. Phys., **19**, 1459-1477 (1951).
[17] A. C. Wahl, P. E. Cade, C. C. J. Roothaan, J. Chem. Phys,. **41**, 2578-2599 (1964).
[18] M. P. Barnett, C. A. Coulson, Phil. Trans. Roy. Soc. London **A 243**, 221-233 (1951).
[19] P. O. Löwdin, Adv. Phys., **5**, 1-172 (1956).
[20] H. J. Silverstone, J. Chem. Phys., **47**, 537-540 (1967); J. Chem. Phys., **45**, 4337-4341 (1966).
[21] H. W. Jones, Int. J. Quantum Chem., **18**, 709-713 (1980); Phys. Rev. **A 30**, 1-4 (1984); J. Comput. Chem., **12**, 1217-1222 (1991).
[22] A. Bouferguene, M. Fares, D. Rinaldi, J. Chem. Phys., **100**, 8156-8168 (1994).
[23] A. W. Niukkanen, Int. J. Quantum Chem., **25**, 941-955 (1984).
[24] E. J. Weniger and E. O. Steinborn, Phys. Rev. **A 29**, 2268-2271 (1984).
[25] E. J. Weniger, J. Math. Phys., **26**, 276-291 (1985).
[26] I. Shavitt, *In: Methods in Computational Physics*, Vol. 2, eds. B. Alder, S. Fernbach and M. Rotenberg, Academic Press, New York, (1963).
[27] E.O. Steinborn and E. Filter, Theoret. Chim. Acta **38**, 273-281 (1975).
[28] W. Magnus, F. Oberhettinger and R. P. Soni, *Formulas and Theorems for the Special Functions of Mathematical Physics*, Springer, New York, (1966).

[29] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra*, Cambridge University, Cambridge, England, (1970).
[30] J. A. Gaunt, Philos. Trans. R. Soc. London, Ser. **A 228**, 192-196 (1929).
[31] E. J. Weniger and E. O. Steinborn, Comput. Phys. Commun., **25**, 149-157 (1982).
[32] H. H. H. Homeier and E. O. Steinborn, mt. J. Quantum Chem., **39**, 625-645 (1991).
[33] J. Grotendorst and E.O. Steinborn, Phys. Rev. **A 38**, 3857-3876 (1988).
[34] E. O. Steinborn and H.H.H. Homeier, Int. J. Quantum Chem. Symp., **24**, 349-363 (1990).
[35] E. Filter and E. O. Steinborn, J. Math. Phys., **21**, 2725-2736 (1980).
[36] M. Reed and B. Simon, *Methods of Modern Mathematical Physics II: Fourier Analysis, Self-Adjointness*, Academic Press, New York, (1975).
[37] F. P. Prosser and C. H. Blanchard, J. Chem. Phys., **36**, 1112-1112 (1962).
[38] M. Geller, J. Chem. Phys., **39**, 853-854 (1963).
[39] M. Weissbluth, *Atoms and molecules*, Academic Press, New York, (1978).
[40] I. S. Gradshteyn, I. M. Ryzhik, *Tables of integrals sums series and products*, Sixth Edt., Academic Press, New York, (2000).
[41] I. I. Guseinov, J. Mol. Sci. (Wuhan, China), **5**, 2, 169-174 (1987).

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