



Applicability of noninteger bessel type orbital basis sets: numerical and analytical approaches

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Abstract

Recently, usefulness of the noninteger principal quantum numbers for Bessel type orbitals was discussed by Weniger in (Adv Quant Chem 83:209–237, 2021). In this study, we analyzed the applicability and numerical accuracy of basis sets of noninteger Bessel type orbitals to electronic structure calculations. Both numerical and analytical approaches are applied to two-electron atomic systems. The results of the numerical test demonstrated the potential of the noninteger values of principal quantum number for the improving of Bessel type functions approach in use of LCAO methods. Nevertheless, the analytical approach is still not suitable and in development and needs to be investigated further. The performance of the presented basis functions is also compared to the numerical Hartree–Fock results.

Keywords Bessel type orbital · Noninteger principal quantum number · LCAO methods · Basis function

1 Introduction

In studies of the electronic structure of many electron systems, the basis sets expansions or LCAO methods are the fundamental for the solution of Hartree–Fock–Roothaan (HFR) and advance correlation methods. One of the major factors of these models that should be considered in performing the LCAO calculations is the selection of basis functions [2–9]. The selection of the most appropriate basis functions for a given problem is significantly important and not always clear how to choose basis set in LCAO approaches. Therefore, many different basis functions have been proposed and applied to various problems in quantum chemistry. During the past decade, there have been also an increasing interest and made many efforts in the construction of alternative and efficient basis functions especially suited for accurate

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calculations of few electron systems [10–18]. As desired features, the correct cusp condition at the origin and exponential decay at infinity are essential as a measure of the quality of calculations for correct description of the wave function [19, 20]. Although Gaussian type orbitals (GTOs) are at a disadvantage, namely improper cusp condition and long-range behavior, it should be emphasized that the majority of calculations of the electronic structure of atoms and molecules have been done using GTOs.

For accurate description of one electron wave functions, a careful choice of basis functions is required in HFR or LCAO methods. It is well known that the natural choice of accurate and reliable basis functions in HFR method is the exponential type orbitals (ETOs). In the HFR approximation, Slater type orbitals (STOs) are the simplest analytical and suitable basis functions among the other ETOs because they represent the correct behavior of the electron-nucleus cusp condition and the exponential decay at large distances [21]. It should be also noted that the quality of one electron wave functions can be easily improved by increasing the number of basis functions in LCAO approaches. Other way to improve the quality of wave functions is modifying the radial part of wave functions. Therefore, there are many modifications that have been proposed on the radial part of wave functions which aim to improve the description of one electron basis functions.

Unfortunately, there are some restrictions on basis functions used in LCAO calculations to avoid computational problems. When one uses LCAO method, the use of complete and orthonormal functions in the approximation led to some restrictions on the radial part of chosen basis functions. It is well known that there have been many efforts to remove these restrictions. There are mainly two ways to remove the restrictions. Firstly, Parr [22] introduced noninteger principal quantum numbers for Slater type orbitals (NSTOs) instead of integer ones STOs in LCAO approaches. Secondly, approach is suggested by Koga and Kanayama [23] in which exponential part of radial basis functions modified by the generalized exponential functions (GETOs). The aim of all these approaches is to fulfill the necessary performance requirements in LCAO calculations.

The more recently, we have also proposed some improvements on STOs and NSTOs functions to increase the efficiency and accuracy of LCAO calculations [24–27]. These works were also extended to Bessel type orbitals (BTOs) [28–30]. BTOs are advantageous in Fourier transform (FT) methods, as pointed out in [31–33] and later emphasized by Weniger [34]. The modifications of BTOs would also have a simple FT, provided the positive exponents are restricted to finite values. Clearly, this type of additional flexibility must lead to variationally improved results as in the case of NSTOs and GETOs. However, we found that in literature there is no study reported related to the use noninteger principal quantum numbers for BTOs (NBTOs).

The aim of this work is to examine the applicability the noninteger principal quantum numbers in BTOs and compare their performances in LCAO calculations. To determine the quality and accuracy of the one electron wave functions, we have calculated total energies of atomic systems using numerical and analytical approaches. Our calculations for the total energy have been restricted to two electron systems. Hartree atomic units are used throughout this work.

2 General definitions and computational method

It is well known that the standard BTOs can be expressed as follows [35, 36]

$$B_{q,l}^m(\zeta; \vec{r}) = N_{ql\zeta} r^l \hat{k}_{q-1/2}(\zeta r) S_l^m(\theta, \phi) \quad (1)$$

here, $N_{ql\zeta}$ and $\hat{k}_{q-1/2}(\zeta r)$ are normalization constant and reduced Bessel function (RBF), respectively. $S_{lm}(\theta, \phi)$ is a complex or real spherical harmonic and the parameter $\zeta > 0$ is a screening constant. The RBF is defined as follow:

$$\hat{k}_{q-1/2}(\zeta r) = e^{-\zeta r} \sum_{i=0}^{q-1} \frac{(q-1+i)!(\zeta r)^{q-i-1}}{(q-1-i)!i!2^i} \quad (2)$$

where q is unconventional indices expressed as $q = n - l$. Here, n and l are the principal and angular quantum numbers, respectively.

Conventional integer BTOs assume that the principal quantum number n in Eq. (1) is positive integer. By removing this restriction on the principal quantum number n , noninteger principal quantum number can be defined as a new variational parameter ν . Hence, noninteger BTOs (NBTOs) can be defined as [1]

$$B_{\nu,l}^m(\zeta; \vec{r}) = N_{\nu l\zeta} r^l \hat{k}_{\nu-1/2}(\zeta r) S_l^m(\theta, \phi) \quad (3)$$

where ν is the variational parameter as used in the NSTOs calculations [22–25]. Here, $N_{\nu l\zeta}$ is the normalization constant and $\hat{k}_{\nu-1/2}(\zeta r)$ is the RBF of arbitrary order ν . In this equation the RBF is defined by the modified Bessel function of second kind, denoted by $K_{\nu-1/2}(\zeta r)$ and ν -th order, with $\nu > 0$. The RBF of arbitrary order ν can also be defined as follow

$$\hat{k}_{\nu-1/2}(\zeta r) = \left(\frac{2}{\pi}\right)^{1/2} (\zeta r)^\nu K_{\nu-1/2}(\zeta r) \quad (4)$$

and where $K_{\nu-1/2}(\zeta r)$ can be expressed as [37]

$$K_{\nu-1/2}(\zeta r) = e^{-\zeta r} \sum_{n=0}^{\infty} \sum_{i=0}^n \lambda(\nu - 1/2, n, i) (\zeta r)^{i-\nu+1/2} \quad (5)$$

with the coefficients

$$\lambda(\nu - 1/2, n, i) = \frac{(-1)^i \sqrt{\pi} \Gamma(2\nu - 1) \Gamma\left(\frac{1}{2} + n - \nu + \frac{1}{2}\right) L(n, i)}{2^{\nu-1/2-i} \Gamma(1 - \nu) \Gamma(n + \nu) n! 2^{\nu+l} \Gamma(\nu + l + 1)} \quad (6)$$

that contain Lah numbers, denoted by $L(n, i)$ satisfying $L(0, 0) = 1$; $L(n, 0) = 0$ and $L(n, 1) = n!$ conditions for $n, i > 0$,

$$L(n, i) = \binom{n-1}{i-1} \frac{n!}{i!} \quad (7)$$

when Eqs. (6, 7) are inserted into Eq. (3), the analytic NBTOs (ANBTOs) can be expressed as follow

$$B_{\nu,l}^m(\zeta;\vec{r}) = N_{\nu,l}(\zeta r)^{l+1} \sqrt{\frac{2}{\pi}} e^{-\zeta r} \sum_{n=0}^k \sum_{i=0}^n \frac{(-1)^i \sqrt{\pi} \Gamma(2\nu-1) \Gamma(1+n-\nu) L(n,i)}{2^{2\nu+l-1/2-i} \Gamma(1-\nu) \Gamma(n+\nu) n! \Gamma(\nu+l+1)} S_l^m(\theta, \phi) \quad (8)$$

The reason is that new NBTOs and ANBTOs is more general than the approach in Eq. (1) due to the extra degree of freedom introduced by the parameter ν . In the analytical expressions ANBTOs obtained, the k value is used to provide practical calculation opportunity instead of the infinite value, which is the upper limit of the sum in the modified Bessel function of second kind in Eq. (5). All the parameters occurring in NBTOs and ANBTOs were variationally optimized with the help of Newton method. To avoid local minimums, optimization process has been performed using different initial values for all nonlinear parameters.

3 Numerical results and discussion

In this study, by the use of NBTOs and ANBTOs within minimal basis sets approximation, the HFR calculations have been performed for the ground states of two electron atomic systems. Both numerical NBTOs and analytic ANBTOs approaches have been applied to atomic HFR calculations. The results of the examination of the usefulness of both approaches have been compared and presented. In order to show the precision and accuracy of NBTOs results, we have been compared the performance between both basis sets and other standard basis sets used in HFR calculations. Some orbital expectation values, energy of isoelectronic systems and ionization potential values have been calculated and compared to other basis sets used in literature and available experimental values for more detail analysis.

Table 1 summarizes the HFR total energies obtained with optimized basis sets of NBTOs for the ground-state atoms and ions: He, H^- and Li^+ systems. As can be seen from this table, the NBTOs total energy results are slightly better than those of conventional BTOs [36] and NSTOs [38] results. Total energy errors with respect to the results of numerical Hartree–Fock (NHF) total energies [39] $\Delta E_{NBTOs-NHF}$ are

Table 1 NBTOs total energies (E_{NBTOs} , signreversed) and total energy differences of NBTOs from the ^aBTOs ($\Delta E_{BTOs-NBTOs}$), the ^bNSTOs ($\Delta E_{NSTOs-NBTOs}$) and ^cNHF ($\Delta E_{NBTOs-NHF}$) results for the ground states of two electron atomic systems (in a.u.)

System	E_{NBTOs}	$\Delta E_{BTOs-NBTOs}$	$\Delta E_{NSTOs-NBTOs}$	$\Delta E_{NBTOs-NHF}$
He	2.85851270	0.01085645	0.00430420	0.00316730
H^-	0.48292042	0.01026417	0.00404618	0.00500932
Li^+	7.23365134	0.01099509	0.00435660	0.00276386

^aBTOs HFR total energy results taken from [36]

^bNSTOs HFR total energy results taken from [38]

^cNHF HFR total energy results taken from [39]

Table 2 Optimum NBTOs parameters; virial ratio (V , sign reversed), noninteger quantum numbers (ν) and screening parameters (ζ) for the ground states of two electron atomic systems

System	ν	ν	ζ
He	2.00000002	0.85768417	1.52187293
H^-	2.00000001	0.72312035	0.55194138
Li^+	2.00000000	0.90460636	2.51268625

Table 3 The NBTOs total energy errors (in mhartree) relative to the a NDSTOs basis sets ($\Delta E_{NBTos-NDSTos}$) for the ground state of two electron atomic systems

Atom	$\Delta E_{NBTos-NDSTos}$
He	3.161
Li^+	2.761

^aNDSTOs HFR total energy results taken from Ref [40]

also given in these tables. It is observed that the errors for the total energies of studied systems are similar with respect to NHF values. The description of the cationic system is more notable. The virial ratio $V = \frac{\langle \hat{V} \rangle}{\langle \hat{T} \rangle}$, optimal noninteger quantum numbers (ν) and the screening parameters (ζ) for NBTOs basis sets are also given in Table 2. Here, the \hat{T} and \hat{V} are the kinetic-energy operator, and the potential energy operator, respectively. We also compared NBTOs results to more effective noninteger double-zeta STOs (NDSTOs) basis set results [40] to analyze the general behavior and the quality of the NBTOs basis sets. In Table 3, we list the difference of total energy results in miliHartree for He and Li^+ systems between the NBTOs and NDSTOs basis sets. Cationic system is again the more accurate one. Unfortunately, there is no enough double-zeta data for ionic systems available yet to compare and determine the quality of NBTOs basis sets.

When we used the ANBTOs as basis functions for HFR calculations, we have analytical approach to compare and increase the computational efficiency of NBTOs. In this approach, to reduce the computational time for the calculation of matrix elements and optimization process in HFR procedure, the summation in Eq. (8) was truncated at some values of $k=2-10$ for the total energy calculation of He atom. The optimized nonlinear parameters have been taken from NBTOs basis sets calculation as $\nu = 0.85768417$ and $\zeta = 1.52187293$. In Table 4, we list the total energy values for He atom to analyze on the behavior of energy convergence and efficiency of computational cost. As can be seen from the Table 4, the convergence of energy values is doubtful and problematic. A much larger expansion for the parameter k is necessary to reach the smoothly converges and get reliable accurate total energy values. Therefore, we also searched the error for convergence behavior in ANBTOs approach. Thus, the convergence behavior has been also checked by the use of two electron and kinetic energy integrals with

Table 4 ANBTOs total energies (E , signreversed), optimized values of noninteger principal quantum numbers (ν) and orbital exponents (ζ) in single-zeta approach for the ground state He atom (in a.u.)

Atom	k	ν	ζ	E
He	2	0.85768417	1.52187293	2.46560769
	3			2.29593363
	4			2.20351887
	5			2.12344552
	6			2.05191448
	7			1.98725627
	8			1.92846539
	9			1.87346298
	10			1.70332016

the same nonlinear parameters $\nu = 0.85768417$ and $\zeta = 1.52187293$ for ANBTOs basis sets. The differences of two electron integral values ΔTEI for ANBTOs basis sets relative to the exact numerical two electron integral values obtained from NBTOs basis sets are given in Table 5. Similarly, the differences of kinetic energy integral values ΔKEI for ANBTOs basis sets relative to the exact numerical kinetic energy integral values obtained from NBTOs basis sets are given in Table 6. Unfortunately, in both cases there are no regular convergence behavior

Table 5 Errors ΔTEI in numerical values of two electron integral for He atom

k	ν	ζ	ΔTEI
2	0.85768417	1.52187293	- 0.39548042
3			- 0.31172811
4			- 0.37397940
5			- 0.42505097
6			- 0.46602445
7			- 0.49966135
8			- 0.52807637
9			- 0.55140008
10			- 0.45231308

Table 6 Errors ΔKEI in numerical values of kinetic energy integral for He atom

k	ν	ζ	ΔKE
2	0.85768417	1.52187293	- 0.51660270
3			- 0.26929703
4			- 0.28634355
5			- 0.30791810
6			- 0.32802799
7			- 0.34623881
8			- 0.36273824
9			- 0.37777375

obtained. The huge fluctuation of the numerical values of integrals must be considered for further research. Therefore, at this moment, there is not enough evidence to support the use of ANBTOs basis sets in HFR calculations.

To further investigate of the applicability and accuracy of NBTOs, some radial expectation values of 1 s orbital $\langle r^k \rangle_{1s}$ ($k = -2, -1, 1, 2$) have been also calculated and compared with the results calculated using the extended basis set of STOs [39] for the ground states of He, H^- and Li^+ . In Table 7, these comparative results are given. Here, extended basis sets of STOs results can be seen as NHF results for orbital moments. Orbital energy results are also given in this table. The NBTOs relative errors with respect to the extended basis sets of STOs showed that the most accurate results can be achieved for the $\langle r^{-1} \rangle$ values. In this table, it was also found that the cation values for the orbital moments are more accurate than anions.

Moreover, the performance of the NBTOs basis sets for the isoelectronic series of He atom is examined. Table 8 summarizes the HFR total energies obtained with optimized basis sets of NBTOs for the ground state of isoelectronic series of He. In order to see the improvement of the proposed NBTOs basis sets, comparison has been made with the NHF results [41]. To more clearly see the effect of NBTOs basis sets among different basis sets used in literature, a more quantitative comparison is also made with results calculated from standard BTOs ($\Delta E_{BTOs-NHF}$) and NSTOs [40] ($\Delta E_{NSTOs-NHF}$) basis sets with respect to NHF values [41]. We should emphasize that the accuracy of the NBTOs ($\Delta E_{NBTOs-NHF}$) basis sets approximately 6 times and 3 times more accurate than the BTOs and NSTOs relative to the NHF values. It is observed that the variation of total energy error relative to the NHF values is negligible when the atomic number increases in isoelectronic series. In addition to this, it is clear to see in Fig. 1 that the effect of noninteger principal quantum number in HFR calculations is significant. The performance of the NBTOs basis sets surpass the basis sets of standard BTOs and the NSTOs as can be seen in Fig. 1.

As a last comparison, as a physical property, ionization potential energy values for isoelectronic series of He atom have been calculated with standard BTOs and NBTOs to see the effectiveness of non-integral principal quantum numbers used in BTOs. The results of comparison with respect to the experimental values [42] are given in Fig. 2. In this case, the NBTOs values are slightly better than the BTOs but not significantly different.

As can be seen from the numerical tables, the NBTOs definition, which achieve double-zeta accuracy, lead to a significant gain in the HFR total energy calculations. The data obtained according to the upper limit k value in Eq. (8) for ANBTOs basis sets should definitely be examined more deeply to determine their applicability in further studies.

Table 7 The orbital energies of NBTOs basis sets (sign reversed), the NBTOs radial expectation values of 1 s orbital (in Bohr) $\langle r^k \rangle_{1s}$ ($k = -2, -1, 1, 2$) and their relative errors (NBTOs-STOs) with respect to the extended basis sets of ^aSTOs results (given in parentheses) for the ground states of two electron atomic systems

System	1 s	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle r^{-1} \rangle$	$\langle r^{-2} \rangle$
<i>H</i> ⁻	0.48292042 (-0.43669802)	2.31929 (-0.18467)	7.4277 (-1.98336)	0.68825 (0.002578)	1.08911 (0.00763)
<i>He</i>	0.91254205 (0.00541395)	0.913483 (-0.01379)	1.13049 (-0.05434)	1.68761 (0.00033)	6.03323 (0.03773)
<i>Li</i> ⁺	2.78785042 (0.00450958)	0.56796 (-0.004407)	0.43455 (-0.010771)	2.68754 (0.00012)	14.9758 (0.06578)

^aHFR orbital energies and radial expectation values obtained with extended basis sets of STOs taken from [39]

Table 8 NBTOs (E_{NBTOs}) total energies (sign reversed) and energy differences of BTOs ($\Delta E_{BTOs-NHF}$), ^aNSTOs ($\Delta E_{NSTOs-NHF}$), NBTOs ($\Delta E_{NBTOs-NHF}$) from the ^bNHF values for the isoelectronic series of He atom (in a.u.)

Atom	Z	E_{NBTOs}	$\Delta E_{BTOs-NHF}$	$\Delta E_{NSTOs-NHF}$	$\Delta E_{NBTOs-NHF}$
He	2	2.858512695	0.014023746	0.007471499	0.0031673
Li ⁺	3	7.233651344	0.013758951	0.007120463	0.0027639
Be ⁺²	4	13.60871185	0.01364318	0.006965295	0.0025876
B ⁺³	5	21.98374558	0.01357822	0.006877785	0.0024889
C ⁺⁴	6	32.35876704	0.01353663	0.006821593	0.0024258
N ⁺⁵	7	44.73378190	0.01350771	0.006782451	0.0023821
O ⁺⁶	8	59.10879278	0.01348645	0.006753633	0.0023499
F ⁺⁷	9	75.48380109	0.01347016	0.00673153	0.0023253
Ne ⁺⁸	10	93.85880765	0.01345727	0.00671402	0.0023059
Na ⁺⁹	11	114.2338130	0.01344685		0.0022901
Mg ⁺¹⁰	12	136.6088173	0.01343775		0.0022771
Al ⁺¹¹	13	160.9838210	0.01343095		0.0022662
Si ⁺¹²	14	187.3588241	0.01342475		0.0022569
P ⁺¹³	15	215.7338268	0.01341935		0.0022488
S ⁺¹⁴	16	246.1088292	0.01341475		0.0022418
Cl ⁺¹⁵	17	278.4838312	0.01341065		0.0022357
Ar ⁺¹⁶	18	312.8588331	0.01340705		0.0022302
K ⁺¹⁷	19	349.2338347	0.01340375		0.0022253
Ca ⁺¹⁸	20	387.6088362	0.01340085		0.0022209

^aNSTOs HFR total energy results taken from [40]

^bNHF HFR total energy results taken from [41]

4 Conclusion

In this work, we comparatively report the accuracy and computational efficiency of NBTOs and ANBTOs approaches in HFR method. The numerical test for two electron system and their isoelectronic series shows the superior performance of the

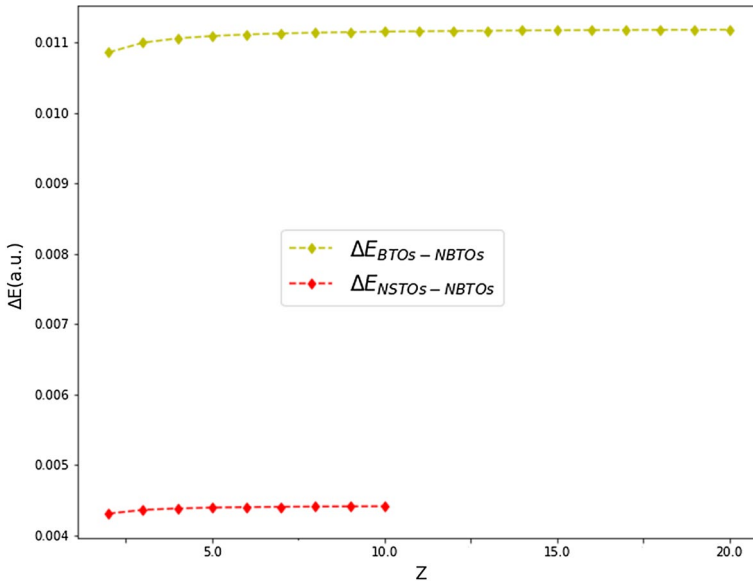


Fig. 1 The energy differences ΔE between E_{BTOs} , E_{NSTOs} [40] and E_{NBTOs} as a function of atomic number Z for the isoelectronic series of He atom

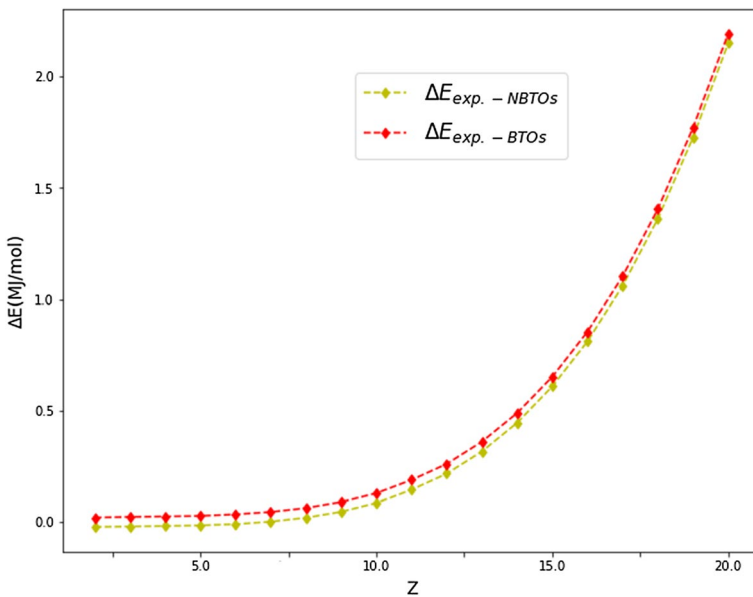


Fig. 2 The ionization potential differences ΔE (in MJ/mol) between E_{NBTOs} , E_{BTOs} and experimental values [42] as a function of atomic number Z for the isoelectronic series of He atom

NBTOs basis sets and its applicability to LCAO approach. The feasibility and the efficiency of the ANBTOs approach also tested. More investigation should be considered on the applicability of analytical approach to reduce the computational cost and extend the applicability of ANBTOs to few electron systems [43, 44].

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Data availability Full details of the resulting wave functions are available by request through e-mail address: merturk@comu.edu.tr.

Declarations

Competing interests The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Ethical approval Not applicable.

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