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Generalized complete orthonormal sets of Exponential-Type functions

G. Demirdak [a], E. Sahin [b], M. Ertürk [a,*]

[a] Department of Physics, Faculty of Sciences, Çanakkale Onsekiz Mart University, 17100 Çanakkale, Türkiye
[b] Taşova Yüksel Akın Vocational School, Amasya University, 05800, Amasya, Türkiye

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ABSTRACT

New generalized complete orthonormal sets of $\psi^{(\alpha^*,\mu)}$-exponential type functions are described and applied to LCAO calculations for the total energies of atomic systems within the framework of the minimal basis sets approximation in combined Hartree-Fock-Roothaan method. A new variational parameter μ is proposed in the complete orthonormal sets of $\psi^{(\alpha^*,\mu)}$-exponential type functions where α^* parameter changes in the range $-\infty < \alpha^* < 3$. The combined Hartree-Fock-Roothaan calculations have been performed to determine the performance of new basis sets. The comparison has been made by the use of different generalized exponential type basis sets used in the literature. The optimal values of parameters are determined by minimizing the total energies. According to obtained total energy results, the $\psi^{(\alpha^*,\mu)}$ basis sets are more effective than standard definition of $\psi^{(\alpha^*)}$ basis sets and there is no restriction on α^* values studied systems in this work.

1. Introduction

Electronic structure calculations of atomic/molecular systems have importance not only energy results but also other physical/chemical properties which can be obtained with the help of quantum mechanical postulates [1]. Thus, linear combination of atomic orbitals (LCAO) based ab initio methods require accurate and effective basis functions. If one pays attention to effectiveness part only, Gaussian type functions become the first choice for the construction of basis sets due to computational advantage of their molecular integrals [2]. On the other hand, it is well known that the exponential type functions (ETFs) better describe electronic wave function in the short range and long range from the nuclei than Gaussians [3].

Slater type functions (STFs) [4], B functions (BTFs) [5] and $\psi^{(\alpha^*)}$ functions ($-\infty < \alpha^* < 3$) [6,7] are commonly used ETFs in the electronic structure calculations. However, searching for modified basis functions takes interest to obtain more flexibility and accuracy in a small basis set. Past research has shown that the total and orbital energies, and orbital moments have improved when exponential part of the non-integer STFs $e^{-\zeta r}$ changed by $e^{-\zeta r^{\mu}}$ within the single-zeta approximation [8]. That new basis function was called noninteger generalized exponential type functions (NGETFs). Recently, this approach was extended to BTFs by replacing r to r^{μ} in the radial part of these functions and hereby generalized BTFs (GBTFs) was introduced [9]. It should be noted that the new parameter μ was less than unity for neutral and singly charged ionic species for both NGETFs and GBTFs. Those results indicate that variational μ parameter brings more flexibility to ETFs when we remove $\mu = 1$ restriction.

Another class of ETFs are the complete orthonormal sets which contain Laguerre polynomials. Hydrogen-like functions [10], Coulomb-Sturmians [11,12] and Lambda functions [13,14] remain attractive for quantum chemical calculations. The $\psi^{(\alpha^*)}$-ETFs with $-\infty < \alpha^* < 3$ are the general form of the complete orthonormal sets of ETFs. All three functions mentioned above can be obtained from $\psi^{(\alpha^*)}$-ETFs in special cases [6]. Atomic and molecular electronic structure calculations were also performed by using $\psi^{(\alpha^*)}$-ETFs as a basis function (for this purpose, the orbital parameter should not be taken the same for all orbitals and should be optimized variationally) [15,16]. The aim of this study is to further extend the applicability of the generalization approach r^{μ} to $\psi^{(\alpha^*)}$-ETFs.

In the next section, we have constructed new generalized ETFs using the parameter μ in the radial part of $\psi^{(\alpha^*)}$ to investigate the effect of unrestricted parameter μ on the atomic orbitals using the atomic Hartree-Fock-Roothaan (HFR) calculations within the minimal basis set approach.

* Corresponding author.
E-mail address: merturk@comu.edu.tr (M. Ertürk).

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Table 1
Total energy of $\psi^{(\alpha^*,\mu)}$−GETFs ($E^{(\alpha^*,\mu)}$, sign reversed), optimal α^* values (in parentheses), total energy differences $\Delta E(X) = E_X - E^{(\alpha^*,\mu)}$ of various basis sets with respect to the $E^{(\alpha^*,\mu)}$ and optimal μ values for neutral systems in a.u.

Atom	$E^{(\alpha^*,\mu)}(\alpha^*)$	$\Delta E(\psi^{(\alpha^*)})$ [a]	$\Delta E(GBTFs)$ [b]	$\Delta E(NGETFs)$ [c]	μ
He	2.86107342 (2.62079903)	0.01341717	0.0	−0.00040392	0.89658230
Be	14.57162364 (2.25029390)	0.01277599	0.02926371	0.00064484	0.95036058
B	24.51917665 (2.25646382)	0.01798957	0.04343541	−0.00413305	0.95401296
C	37.65601691 (2.24467537)	0.03036621	0.0604730	−0.01820189	0.95173207
N	54.3261407 (2.21201688)	0.05365831	0.08154518	−0.0440071	0.94679043
O	74.64396059 (2.12682813)	0.0993857	0.11121647	−0.09704611	0.93851206
F	99.11786883 (2.04244555)	0.17103758	0.14703257	−0.16722027	0.93045075
Ne	128.09320665 (1.95935300)	0.27588436	0.18966685	−0.25378035	0.92285704
Mg	199.13019496 (2.31353254)	0.29638056	0.19004276	−0.31396204	0.93668529
Ar	525.72377154 (2.65987703)	0.35260718	0.48493004	−0.92323846	0.95599724
Ca	675.52356785 (2.48139801)	0.34013423	0.04680625	−1.07225315	0.95782679

[a] $\psi^{(\alpha^*)}$-ETFs total energy results taken from Ref.[15].
[b] GBTFs total energy results taken from Ref.[9].
[c] NGETFs total energy results taken from Ref.[8].

Table 2
Total energy of $\psi^{(\alpha^*,\mu)}$−GETFs ($E^{(\alpha^*,\mu)}$, sign reversed), optimal α^* values (in parentheses), total energy differences $\Delta E(X) = E_X - E^{(\alpha^*,\mu)}$ of various basis sets with respect to the $E^{(\alpha^*,\mu)}$ and optimal μ values for anions in a.u.

Anion	$E^{(\alpha^*,\mu)}(\alpha^*)$	$\Delta E(GBTFs)$ [a]	$\Delta E(NGETFs)$ [b]	μ
Li^-	7.424921473 (2.99000000)	0.003509823	−0.00052993	0.93222176
B^-	24.47702853 (2.51388131)	0.02644651	−0.02249347	0.94668097
C^-	37.6183898 (2.46135432)	0.03982723	−0.05093120	0.94257926
N^-	54.12625472 (2.33286111)	0.06131084	−0.10934028	0.93443393
O^-	74.45074371 (2.21598216)	0.08820719	−0.18616199	0.92600257
F^-	98.9384949 (2.10524916)	0.05435567	−0.28045130	0.91790485
Na^-	161.34532554 (2.49266067)	0.10209284	−0.32733646	0.9334535
Cl^-	458.45135153 (2.83995773)	0.00080563	−0.94195647	0.95485522
K^-	597.99436777 (2.53921215)	0.17310987	−1.00172223	0.95731869

[a] GBTFs total energy results taken from Ref.[9].
[b] NGETFs total energy results taken from Ref.[8].

2. General definitions and computational details

The $\psi^{(\alpha^*)}$-ETFs used in literature are defined as [7]

$$\boldsymbol{\psi}^{(\boldsymbol{\alpha}^*)}_{\boldsymbol{nlm}}(\boldsymbol{\zeta},\vec{\boldsymbol{r}}) = \frac{(2\boldsymbol{\zeta})^{\frac{3}{2}}}{\Gamma(\boldsymbol{p}^*+1)}\left(\frac{\Gamma(\boldsymbol{q}^*+1)}{(2\boldsymbol{n})^{\boldsymbol{\alpha}^*}[\boldsymbol{n}-\boldsymbol{l}-1]!}\right)^{\frac{1}{2}} \boldsymbol{e}^{-\frac{\mathbf{x}}{2}}\mathbf{x}^{\boldsymbol{l}}{}_1F_1(-[\boldsymbol{n}-\boldsymbol{l}-1];\boldsymbol{p}^*+1;\mathbf{x})\boldsymbol{S}_{\boldsymbol{lm}}(\boldsymbol{\theta},\boldsymbol{\varphi}) \tag{1}$$

where $\boldsymbol{n},\boldsymbol{l}$ and $\boldsymbol{m}$ are principal quantum number, angular momentum quantum number and magnetic quantum number, respectively. The related quantities are expressed as $\boldsymbol{p}^* = 2\boldsymbol{l}+2-\boldsymbol{\alpha}^*$, $\boldsymbol{q}^* = \boldsymbol{n}+\boldsymbol{l}+1-\boldsymbol{\alpha}^*$, $-\infty < \alpha^* < 3$, $0 < \boldsymbol{\zeta} < \infty$, and $\mathbf{x} = 2\zeta\mathbf{r}$. ${}_1F_1$ and $\Gamma(\boldsymbol{x})$ are the confluent hypergeometric function and gamma function, respectively. The functions $S_{lm}(\theta,\varphi)$ are the complex or real spherical harmonics defined in Ref. [6,15]. The $\boldsymbol{\psi}^{(\alpha^*)}$-ETFs satisfy the following orthonormality relation:

$$\int \psi^{(\alpha^*)\,\dagger}_{nlm}(\zeta,\vec{r})\left(\frac{2n}{x}\right)^{(\alpha^*)}\psi^{(\alpha^*)}_{n'l'm'}(\zeta,\vec{r})d^3\vec{r} = \delta_{nn'}\delta_{ll'}\delta_{mm'} \tag{2}$$

However, there are still some restrictions on radial part of $\psi^{(\alpha^*)}$-ETFs in eq. (1). Therefore, the exponential part of radial basis functions can be further improved by replacing the radial variable r^μ in $\psi^{(\alpha^*)}$-ETFs. Thus, the $\psi^{(\alpha^*)}$-ETFs gain additional flexibility to represent the atomic orbital

Table 3
Total energy of $\psi^{(\alpha^*,\mu)}$−GETFs ($E^{(\alpha^*,\mu)}$, sign reversed), optimal α^* values (in parentheses), total energy differences $\Delta E(X) = E_X - E^{(\alpha^*,\mu)}$ of various basis sets with respect to the $E^{(\alpha^*,\mu)}$ and optimal μ values for cations in a.u.

Cation	$E^{(\alpha^*,\mu)}(\alpha^*)$	$\Delta E(GBTFs)$ [a]	$\Delta E(NGETFs)$ [b]	μ
Li^+	7.235939588 (2.82187202)	0.0	−0.00031654	0.93398584
B^+	24.23665965 (1.96052539)	0.06669457	0.00121275	0.96072038
C^+	37.28382426 (2.01885565)	0.08599958	−0.00290084	0.96043141
N^+	53.85932847 (2.03532656)	0.10954368	−0.0155484	0.95660442
O^+	74.30604211 (2.02563384)	0.13795158	−0.0389781	0.95117726
F^+	98.68358236 (1.96714714)	0.17605252	−0.0876742	0.94290991
Ne^+	127.55552033 (1.90545442)	0.22078773	−0.152350	0.93510225
Na^+	161.26660133 (1.84241927)	0.27266703	−0.232448	0.92783639
Al^+	241.21437707 (2.14347634)	0.43539467	0.298249	0.93971076
K^+	597.94207395 (2.50605678)	0.25802105	−0.912458	0.95693054
Sc^+	758.23857676 (2.49382882)	–	−1.115708	0.96110548

[a] GBTFs total energy results taken from Ref.[9].
[b] NGETFs total energy results taken from Ref.[8].

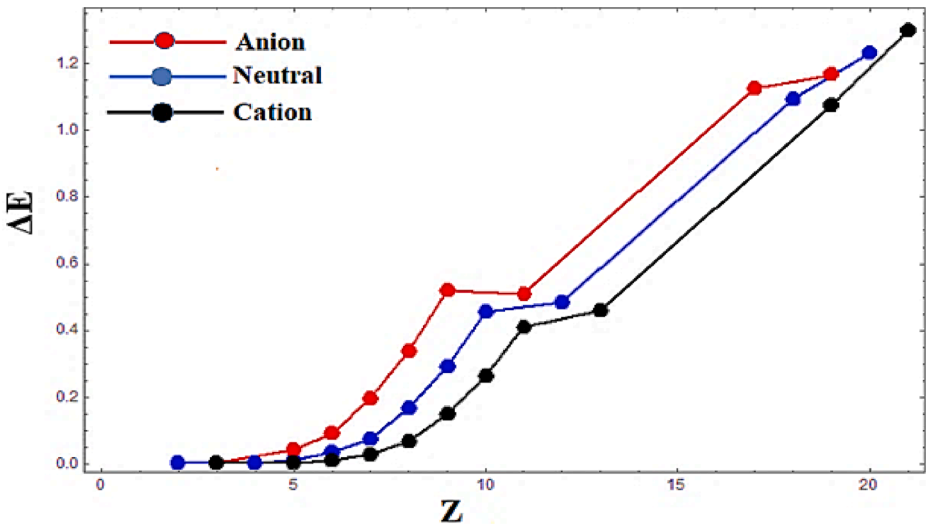


Fig. 1. The energy differences ΔE between $E^{(\alpha^*,\mu)}$ and E_{NHF} [25,26] as a function of atomic number Z for the ground state of neutral atoms and their ions (in au).

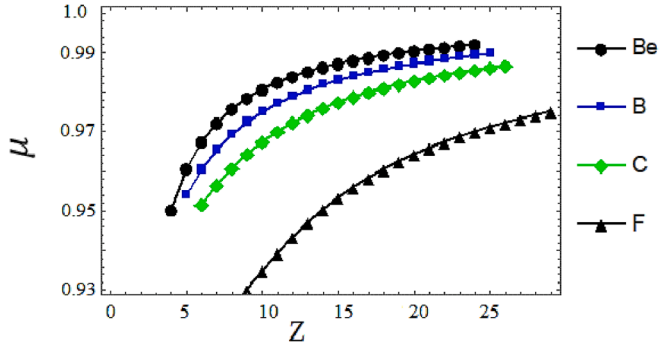


Fig. 2. The variation of optimal μ values as a function of atomic number Z for the isoelectronic series of Be, B, C, and F atoms.

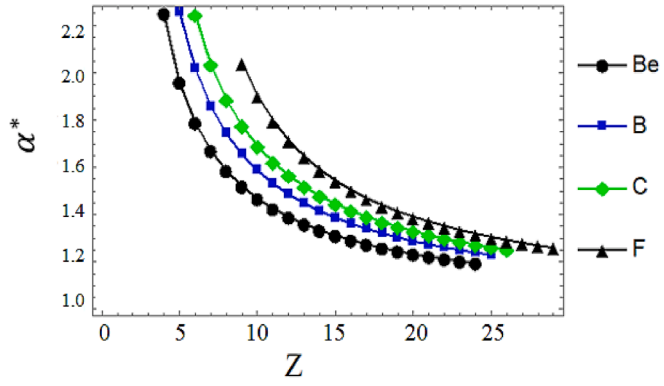


Fig. 3. The variation of optimal α^* values as a function of atomic number Z for the isoelectronic series of Be, B, C, and F atoms.

correctly. Therefore, new radial part of generalized $\psi^{(\alpha^*,\mu)}$-ETFs ($\psi^{(\alpha^*,\mu)}$-GETFs) can be defined in this study as

$$R_{nl}^{(\alpha^*,\mu)}(\zeta,r)=\frac{(2\zeta)^{\frac{3}{2}}}{\Gamma(p^*+1)}\left(\frac{\Gamma(q^*+1)}{(2n)^{\alpha^*}[n-l-1]!}\right)^{\frac{1}{2}}e^{-\frac{x}{2}}x^{l}{}_1F_1(-[n-l-1];p^*+1;x) \tag{3}$$

Here, $x=2\zeta r^{\mu}$ and μ is the additional variational parameters. To avoid the computational difficulties in HFR calculations, the nonlinear parameter μ was chosen to be common for all the $\psi^{(\alpha^*,\mu)}$-GETFs in an atomic system. It should be noted that the Lambda and Coulomb-Sturmian ETFs introduced in Refs. [17–20] are the special cases of the $\psi^{(\alpha^*)}$-ETFs for $\alpha^*=0$ and $\alpha^*=1$, respectively. In order to generalize these well-known ETFs with approach given in eq. (3), one can also define generalized Lambda and Coulomb-Sturmian ETFs to make the constructed basis functions more efficient in performance when HFR methods are employed. As another important feature, it should be also point out that all the ETFs can be written as finite linear combinations of other ETFs to simplify the calculations of matrix elements in LCAO method [6,15].

In this work, we used combined HFR (CHFR) method was mainly described in Refs. [21–22]. For the open shell cases, the coupling projection coefficients have been taken from Refs. [23]. The nonlinear parameters used in $\psi^{(\alpha^*,\mu)}$-GETFs were variationally optimized with the help of Newton method. Using many different initial values in optimization process, orbital-dependent CHFR total energy functional has been minimized to find the optimal values of parameters. As a starting point, the initial values of the nonlinear parameters were taken from the $\psi^{(\alpha^*)}$-ETFs results [15,24]. In all calculations, the deviation of virial ratios from the desired theoretical value -2 for $\psi^{(\alpha^*,\mu)}$-GETFs is about 1×10^{-7}.

3. Results and discussion

Self-consistent field LCAO calculations have been carried out by the use of proposed $\psi^{(\alpha^*,\mu)}$-GETFs basis sets given in this study within the minimal basis sets framework for some atomic and ionic systems. The $\psi^{(\alpha^*,\mu)}$-GETFs HFR total energy values ($E^{(\alpha^*,\mu)}$) are provided in Table 1 with comparison to the total energies of GBTFs $\Delta E(GBTFs)$ and NGETFs $\Delta E(NGETFs)$. The parameters α^* in parentheses and μ for $\psi^{(\alpha^*,\mu)}$-GETFs are also given in this table. As can be seen from Table 1, the total energy values of $\psi^{(\alpha^*,\mu)}$-GETFs are better than the GBTFs result but still significantly deteriorate when comparing NGETFs results as atomic number increases. This is because of the efficiency of noninteger principal quantum number used in NGETFs basis sets. We also observed that the optimal α^* parameter range is between 2 and 3. As pointed out in Ref. [15], the best optimal integer value of $\alpha^*=2$ and noninteger value of α^* have reached to upper limit value 3 with increasing atomic number. Therefore, the restriction on α^* was caused negative effect on total energy minimization. However, the optimal parameter α^* in $\psi^{(\alpha^*,\mu)}$-GETFs cannot reach the maximum value restricted as $\alpha^*<3$. Therefore, optimization of $\psi^{(\alpha^*,\mu)}$-GETFs parameters in HFR total energy

calculations have been completed safely without any restriction. This is the reason why the $\psi^{(\alpha^*,\mu)}$-GETFs basis sets are more effective than $\psi^{(\alpha^*)}$-ETFs as the atomic number increases. In addition to these, one of the important observations is that the optimal value of parameter μ approaches towards the 1 and this trend is a common feature for neutral atom and their ions studied here. Moreover, the optimal μ values increase with increasing atomic number as well. It should be noted that the optimal μ values and their deviations from unity are similar to those observed in Refs. [8,9].

Tables 2 and 3 show the $\psi^{(\alpha^*,\mu)}$-GETFs HFR total energies, the parameters α^* in parentheses and μ for some low-lying states of anions and cations. In these tables, comparative values relative to the total energies of GBTFs $\Delta E(GBTFs)$ and NGETFs $\Delta E(NGETFs)$ are also given. It should be also noted that the optimal μ values in the case of light systems are far from the nominal value of 1. The performance of the $\psi^{(\alpha^*,\mu)}$-GETFs basis sets in the total energy calculations of anions and cations are very similar. Therefore, to distinguish the efficiency of $\psi^{(\alpha^*,\mu)}$-GETFs basis sets in neutral atoms, anions and cations, the total energy errors (ΔE) of the $\psi^{(\alpha^*,\mu)}$-GETFs basis sets with respect to the numerical Hartree-Fock (NHF) values have been plotted in Fig. 1. As can be seen from this figure, the total energy error increases significantly with an increasing atomic number for all systems studied here. We can also conclude that the performance of $\psi^{(\alpha^*,\mu)}$-GETFs basis sets for cationic systems is slightly better than neutral and anions.

To understand the general trend for the parameters α^* and μ, their optimal values are plotted as a function of atomic number in Be, B, C, and F isoelectronic series in Figs. 2 and 3. The calculation results of total energy for the isoelectronic series are given in Tables S1-S4 of the Supporting Information. For the parameter μ, minimum values are always found for minimum value of atomic number in each isoelectronic series. The μ value also increase smoothly towards unity as the atomic number increases in each isoelectronic series. As we can see from Fig. 2 and the tables, the role of the optimal μ value is more important when the heavy atomic system studied. On the other hand, the optimal values for the parameter α^* have reached the maximal values for the lower atomic number in isoelectronic series of systems studied here. The general behavior of the parameter α^* is depicted in Fig. 3. As one can notice from this figure, the parameter α^* value also decrease smoothly as the atomic number increases in each isoelectronic series. The maximum value of the parameter α^* does not exceed the upper limit value of $\alpha^* < 3$.

4. Conclusion

The aim of this study is to show efficiency of proposed $\psi^{(\alpha^*,\mu)}$-GETFs in LCAO method within the minimal basis sets approach. This work is focused on the quality of $\psi^{(\alpha^*,\mu)}$-GETFs with variation of optimal parameters α^* and μ over other similar ETFs used in literature. Unlike the standard definition of $\psi^{(\alpha^*)}$-ETFs in previous work [15], the optimal values of parameter α^* is inherently remained their limit of constraint $-\infty < \alpha^* < 3$. It is found that the $\psi^{(\alpha^*,\mu)}$-GETFs total energies are sufficient to provide more accurate energies than standard definition of $\psi^{(\alpha^*)}$-ETFs. We believe that the $\psi^{(\alpha^*,\mu)}$-GETFs may also play an important role in providing accurate position and momentum space properties. Therefore, in the near future, we will also perform such a comparative analysis for these properties.

CRediT authorship contribution statement

G. Demirdak: Investigation, Formal analysis, Data curation. **E. Sahin:** Investigation, Writing-review& editing. **M. Ertürk:** Conceptulization, Data curation, Supervison, Writing-review& editing.

Declaration of Competing Interest

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.

Data availability

Data will be made available on request.

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Appendix A. Supplementary material

Supplementary data to this article can be found online at https://doi.org/10.1016/j.chemphys.2023.111893.

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