Hartree-Fock-Roothaan Calculations for Ground States of Some Atoms Using Minimal Basis Sets of Integer and Noninteger *n*-STOs

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Hartree-Fock-Roothaan (HFR) calculations for ground states of some atoms, *i.e*. He, Be, Ne, Ar, and Kr have been performed using minimal basis sets of Slater type orbitals (STOs) with integer and noninteger principal quantum numbers (integer *n*-STOs and noninteger *n*-STOs). The obtained total energies for these atoms using minimal basis sets of integer *n*-STOs are in good agreement with those in the previous literature. On the other hand, for the case of minimal basis sets of noninteger *n*-STOs, although the calculated total energies of these atoms agree well with the results in literature, some striking results have been obtained for atoms Ar and Kr. Our computational results for the energies of atoms Ar and Kr are slightly better than those in literature, by amount of 0.00222 and 0.000054 a.u., respectively. The improvement in the energies of atoms Ar and Kr may result from the efficient calculations of one-center two-electron integrals over noninteger *n*-STOs. For some atomic ions in their ground state, HFR calculations have been carried out using minimal basis sets of noninteger *n*-STOs. The obtained total energies for these atomic ions are substantially lower than those available in literature.

Keywords   Hartree-Fock-Roothaan, Slater type orbital

Introduction

The selection of a suitable basis function is of prime importance in the construction of wave functions for atoms and molecules. The commonly used basis functions in Hartree-Fock-Roothaan (HFR) methods are Gaussian Type orbitals (GTOs) and Slater type obitals (STOs). GTOs are extensively used in molecular calculations because their multicenter integrals can be calculated easily. However, it is well-known that STOs yield better convergence of the variational wave functions than GTOs since they possess the singularities of the solution of Schrödinger equation, namely, cusp at nuclei[1] and exponential decay at large distances.[2]

On the other hand, multicenter molecular integrals over STOs are difficult to calculate. Due to the huge advance in computer technology and applied mathematics, the use of STOs in molecular electronic structure calculations has drawn great attention from several groups.[3-8] The studies by these groups are limited to the use of STOs with integer principal quantum numbers (integer *n*-STOs), however.

As is well-known from the literature STOs with noninteger principal quantum numbers (noninteger *n*-STOs) provide better atomic energies than usual STOs.[9] The problem in using noninteger *n*-STOs is the efficient calculation of multicenter integrals. Multicenter integrals over noninteger *n*-STOs are evaluated, especially, by means of Fourier transform convolution

theorem[9b,i,j,k] which is not very well adapted to practical use. Therefore, an efficient algorithm for the evaluation of multicenter integrals over noninteger *n*-STOs has to be developed.

Recently, we have presented an efficient algorithm for the evaluation of two-center overlap and two- and three-center nuclear attraction integrals[10] and multielectron multicenter molecular integrals over noninteger *n*-STOs.[11]

The purpose of this work is to calculate the ground state energy of some closed shell atoms, *i.e*. He, Be, Ne, Ar, and Kr using minimal basis sets of integer and noninteger *n*-STOs, based on the formulae we presented for one-center overlap, nuclear attraction and kinetic energy, and one-center two-electron integrals over noninteger *n*-STOs.

Atomic units (a.u.) will be used throughout this paper.

Computational methods

In this work we used real STOs as basis sets which are defined in the most general case by

$$\chi_{nlm}(\zeta, \vec{r}) = \frac{(2\zeta)^{n+\frac{1}{2}}}{\sqrt{\Gamma(2n+1)}} r^{n-1} \exp(-\zeta r) S_{lm}(\theta, \varphi)$$

(1)

Slater type orbitals

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where ζ is orbital exponent, $S_{lm}(\theta,\varphi)$ is real spherical harmonics and Γ is gamma function.[12]

In the HFR equations of atoms, two types of integrals arise, namely, one-electron one-center integral and two-electron one-center integral.

Types of one-center integrals arising in atomic RHF calculations with noninteger n-STOs are as follows:

Overlap integral,

$$
S_{nlm,n'l'm'}(\zeta,\zeta') = \int \chi_{nlm}^{*}(\zeta,\vec{r})\chi_{n'l'm'}(\zeta',\vec{r})dV =
$$

$$
\frac{\Gamma(n+n'+1)}{\sqrt{\Gamma(2n+1)\Gamma(2n'+1)}}(1+t)^{n+\frac{1}{2}}(1-t)^{n'+\frac{1}{2}}\delta_{ll'}\delta_{mm'}
$$

$$(2)$$

in which $t=(\zeta-\zeta')/(\zeta+\zeta')$ and δ_{ij} is kronecker delta function.

Nuclear attraction integral

$$
U_{nlm,n'l'm'}(\zeta,\zeta') = \int \chi_{nlm}^{*}(\zeta,\vec{r})\frac{1}{r}\chi_{n'l'm'}(\zeta,\vec{r})dV
$$

$$
= \frac{2\zeta'}{\sqrt{2n'(2n'-1)}}S_{nlm,(n'-1)l''m'}(\zeta,\zeta')
$$

$$(3)$$

Kinetic energy integral

$$
T_{nlm,n'l'm'}(\zeta,\zeta') =
$$

$$
-\frac{1}{2}\int \chi_{nlm}^{*}(\zeta,\vec{r})\nabla^2 \chi_{n'l'm'}(\zeta',\vec{r})dV = -\frac{1}{2}\zeta'^2 \bullet
$$

$$
\left(
\begin{array}{c}
S_{nlm,n'l'm'}(\zeta,\zeta') - 2\sqrt{\dfrac{2n'}{2n'-1}}S_{nlm,(n'-1)l'm'}(\zeta,\zeta') + \\[3mm]
\dfrac{4(n'+l')(n'-l'-1)}{\sqrt{2n'(2n'-1)(2n'-2)(2n'-3)}}S_{nlm,(n'-2)l'm'}(\zeta,\zeta')
\end{array}
\right)
$$

$$(4)$$

One-center two-electron integral

$$
C_{n_1 l_1 m_1, n_1' l_1' m_1', n_2 l_2 m_2, n_2' l_2' m_2'}(\zeta_1 \zeta_1', \zeta_2 \zeta_2')
$$

$$
= \int \chi_{n_1 l_1 m_1}^{*}(\zeta_1,\vec{r}_{a1})\chi_{n_1' l_1' m_1'}^{*}(\zeta_1',\vec{r}_{a1})\frac{1}{r_{12}} \bullet
$$

$$
\chi_{n_2 l_2 m_2}(\zeta_2,\vec{r}_{a2})\chi_{n_2' l_2' m_2'}(\zeta_2',\vec{r}_{a2})dV_1 dV_2
$$

$$
= N_{n_1 n_1'}(\zeta_1,\zeta_1') N_{n_2 n_2'}(\zeta_2,\zeta_2') \bullet
$$

$$
\sum_{L,M} A_{m_1 m_1'}^{M} C^{L|M|}(l_1 m_1, l_1' m_1') \bullet
$$
$$
A_{m_2 m_2'}^{M} C^{L|M|}(l_2 m_2, l_2' m_2') R_{N_1 N_1}^{L}(z_1,z_2)
$$

$$(5)$$

where

$$
N_1 = n_1 + n_1', \ N_2 = n_2 + n_2',
$$

$$
z_1 = \zeta_1 + \zeta_1', \ z_2 = \zeta_2 + \zeta_2',
$$

$$
N_{nn'}(\zeta,\zeta') = \frac{(2\zeta)^{n+\frac{1}{2}}}{\sqrt{\Gamma(2n+1)}}\frac{(2\zeta')^{n'+\frac{1}{2}}}{\sqrt{\Gamma(2n'+1)}}
$$

$$(6)$$

and the range of the summation indices L and M are as follows

$$
\max\left[\left|l_1-l_1'\right|,\left|l_2-l_2'\right|\right] \leqslant L \leqslant \min\left[l_1+l_1', l_2+l_2'\right],
$$

$$
-L \leqslant M \leqslant L
$$

$$(7)$$

In Eq. (5), the quantity $C^{L|M|}(lm,l'm')$ and $A_{mm'}^{M}$ are defined in Ref. 3a and the quantity $R_{N_1 N_2}^{L}(z_1,z_2)$ is the integral of the form

$$
R_{N_1 N_2}^{L}(z_1,z_2) = \int_0^\infty r_1^{N_1} e^{-z_1 r_1}\left(\int_0^\infty r_2^{N_2} e^{-z_2 r_2}\frac{r_<^L}{r_>^{L+1}}dr_2\right)dr_1 \quad (8)
$$

which can be calculated as follows

$$
R_{N_1 N_2}^{L}(z_1,z_2) =
$$

$$
\frac{\Gamma(N_1+N_2+1)}{z^{N_1+N_2+1}}\left[
\begin{array}{c}
\dfrac{{}_2F_1(1,N_1+L+2,N_1+N_2+1,z_1/z)}{\Gamma(N_1+L+2)} \\[3mm]
+ \dfrac{{}_2F_1(1,N_2+L+2,N_1+N_2+1,z_2/z)}{\Gamma(N_2+L+2)}
\end{array}
\right] \quad (9)
$$

where ${}_2F_1(a,b,c,x)$ are Hypergeometric functions.[12]

The accuracy of HFR calculations with noninteger n-STOs depends on the efficient evaluation of the one-center Coulomb integrals.

Computational details

In this work, all the integrals appearing in the HFR equations of atoms are calculated on Pentium II by constructing computer programs in Turbo Pascal 7.0 programming language and the accuracy is approximately in the range of 10^{-20}—10^{-25}. One-center two-electron integrals have been calculated by using Eq. (5) which has been tested for wide range of molecular parameters. Here, tridiagonalization procedure was used for diagonalization of Fock matrix.

Molecular wave function parameters (Table 1) for the atoms studied here were taken from the literature: for minimal basis set of integer n-STOs calculations the data in Ref. 13b were used and for minimal basis set of noninteger n-STOs the data in Ref. 14c were used.

Results and discussion

On the basis of the formulae presented here and our

recent works, ground state total energies of some closed shell atoms have been calculated within HFR framework using minimal basis sets of integer and noninteger n-STOs.

In the calculations, the efficient evaluations of two-center one-electron and one-center two-electron integrals were needed. For integer n-STOs, both one-center one- and two-electron integrals are easy to evaluate. However, the computation of one-center two-electron integrals over noninteger n-STOs is rather demanding. In this work, the formula for one-center

two-electron integrals over noninteger n-STOs has been tested extensively for wide range of atomic parameters. Also, in Table 2, some values of one-center two-electron integrals are listed with no comparison due to the scarcity of the numerical values in literature. The values in Table 2 for one-center two-electron integrals over noninteger n-STOs have been tested with the limit values of integer n-STOs and 18-decimal digit accuracy has been achieved.

Using the computer programs constructed for molecular integrals, the calculated HFR total energies of

Table 1 Wave functions for the ground states of atoms He, Be, Ne, Ar, and Kr

Atom	He		Be		Ne		Ar		Kr	
Basis function	Integer n-STOs	Noninteger n-STOs	Integer n-STOs	Noninteger n-STOs	Integer n-STOs	Noninteger n-STOs	Integer n-STOs	Noninteger n-STOs	Integer n-STOs	Noninteger n-STOs
n_{s1}	1	0.955057	1	0.979651	1	0.991639	1	0.995060	1	0.997687
ζ_{s1}	1.6875	1.611725	3.6848	3.611609	9.6421	9.555679	17.5075	17.512938	35.2316	35.483670
n_{s2}			2	2.199546	2	2.109526	2	2.476905	2	2.650223
ζ_{s2}			0.9560	1.048176	2.8792	3.044593	6.1152	7.516514	13.1990	17.599108
n_{s3}							3	2.596234	3	3.111484
ζ_{s3}							2.5856	2.293547	7.0109	7.141756
n_{s4}									4	2.729485
ζ_{s4}									2.8289	2.100332
n_{p1}					2	1.585424	2	1.814212	2	1.916506
ζ_{p1}					2.8792	2.282325	7.0041	6.293187	16.0235	15.219358
n_{p2}							3	2.226151	3	2.783513
ζ_{p2}							2.2547	1.722174	6.8114	6.378034
n_{p3}									4	2.396934
ζ_{p3}									2.4423	1.561459
n_{d1}									3	2.272543
ζ_{d1}									6.8753	5.188147

Table 2 The computer values of two-center one-electron integrals over noninteger n-STOs (in a.u.)

n_1	l_1	m_1	n_1'	l_1'	m_1'	n_2	l_2	m_2	n_2'	l_2'	m_2'	ζ_1	ζ_1'	ζ_2	ζ_2'	Eq. (5)
2.9	1	1	2.5	1	1	5.5	2	1	3.5	2	1	1.61	2.60	6.10	2.30	3.48392359739911513E−01
0.9	0	0	2.7	0	0	2.6	2	1	2.4	2	1	53.47	27.85	11.35	3.65	3.88978496659734 10E−01
2.9	2	2	2.7	2	2	2.2	2	0	1.8	2	0	10.98	1.31	9.82	1.55	1.95123836525682 27E−02
1.7	1	1	1.5	1	1	2.3	2	0	1.9	2	0	4.98	1.27	9.82	1.55	1.43112743483921 19E−01
1.8	1	−1	1.6	1	−1	2.1	2	1	3.9	2	1	4.87	7.52	8.29	6.55	1.04329362146673 49E+00
3.5	3	2	4.5	2	2	5.5	3	1	2.8	2	1	4.57	6.52	3.29	4.55	3.58101940632340 64E−02
6.5	3	1	8.5	3	1	5.8	3	2	2.8	3	2	2.75	2.56	8.92	5.54	2.70267088339633 97E−01
7.8	2	2	6.5	2	2	6.8	2	2	7.4	2	2	3.75	2.84	5.67	6.48	4.63987206299506 85E−01
5.2	2	1	5.4	2	1	4.3	1	1	4.5	1	1	0.65	0.87	9.45	8.56	1.27315778943629 83E−01
4.6	3	3	6.4	3	3	5.4	3	3	3.7	3	3	1.85	2.58	5.52	3.48	4.01360086840795 11E−01
3.5	1	0	2.8	1	0	2.4	0	0	3.4	0	0	0.08	0.05	0.04	0.07	1.33819487749220 83E−02

Table 3   Ground state energies of some closed shell atoms (in a.u.)

Atom	This work		Hartree-Fock[*]
	Integer n-STOs	Noninteger n-STOs	
He	−2.84765625000000	−2.85420849702552	−2.861679996
Be	−14.5567398577072	−14.5642517231389	−14.57302317
Ne	−127.812180939758	−128.298751666422	−128.5470981
Ar	−525.765253605873	−526.589917170338	−526.8175128
Kr	−2744.51962192717	−2750.82871594311	−2752.054977

[*] Hartree-Fock energies for the ground states of these atoms are taken from Ref. 15.

these atoms are listed in Table 3 for both integer n-STOs and noninteger n-STOs. The numeric HF values are also added to Table 3 for comparison.

Our results for the case of integer n-STOs agree well with the previous literature.[13] Moreover, the obtained total energies for the atoms He, Be, Ne, Ar, and Kr using minimal basis set of noninteger n-STOs agree well with the results of Koga, except for atoms Ar and Kr. Our results are slightly better than those of Koga *et al.*[14c] by amounts of 0.00222 a.u. for Ar and 0.000054 a.u. for Kr.

It was also observed that the d-orbital energies of atoms Ar and Kr are positive for basis set of integer n-STOs whereas the use of basis set of noninteger n-STOs will change them to physically realistic negative orbital energies. The relative error was also investigated in energies with respect to numerical HF values (Figure 1). It can be seen from Figure 1 that the relative energy error with respect to HF limits grows by increasing atomic numbers. Meanwhile, it should be noted that total energy improvement does not always increase by increasing atomic number Z.
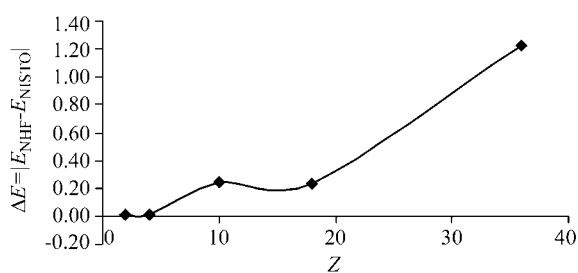
Figure 1   Total energy errors with respect to the HF limit.

Ground state energies of some atomic ions, such as H^-, Be^{2+}, B^{3+}, C^{4+}, N^{5+}, O^{6+}, F^{7+}, Ne^{8+} and Na^{9+} have been calculated using minimal basis set of noninteger n-STOs in HFR approximation (Table 4). It is seen from Table 4 that the obtained total energies are superior to those of Saturno and Parr.[9f] The discrepancies between our results and those of Koga for ground state of neutral atoms and those of Saturno and Parr for atomic ions may result from the more accurate calculation of two-electron one-center integrals and huge advance in computer technology. Note that an error in the range of 10^{-6}—10^{-8} will deteriorate the energy by an amount of

10^{-3} a.u. In all the calculations presented here, Virial coefficients do not deviate from the exact value (-2) by more than 1×10^{-7} which means that our calculations are sufficiently accurate.

Table 4   Energies of some atomic ions (in a.u.)

Atom	This work	Ref. 9f
H^-	−4.78873918637182E−1	−0.4727
Be^{2+}	−1.36043276000311E+1	−13.5977
B^{3+}	−2.10793565804105E+1	−21.9727
C^{4+}	−3.23543706866974E+1	−32.3476
N^{5+}	−44.7293807706675E+1	−44.7227
O^{6+}	−5.91043649498902E+1	−59.0976
F^{7+}	−7.54793862109695E+1	−75.4725
Ne^{8+}	−9.38543843058461E+1	−93.8474
Na^{9+}	−1.14229345606935E+2	−114.223

As is well-known, in molecular calculations, the accuracy in energies of atoms, molecules, clusters and solids is achieved by using extended basis functions. The use of extended basis functions needs more molecular integrals to be evaluated. That is, the calculation of these molecular integrals would require more and more CPU time. It is understood from this work that the use of minimal basis sets of noninteger n-STOs is advantageous over minimal basis sets of integer n-STOs. Namely, lower energies can be obtained using minimal basis sets of noninteger n-STOs instead of minimal basis sets of integer n-STOs. As a conclusion, it can be stated that minimal basis sets of noninteger n-STOs can be used in semi-empirical and density functional studies of heavy atoms, large molecules and clusters, due to the advantage of minimal basis sets of noninteger n-STOs as shown here.

Work is in progress in our laboratory for the calculation of open shell atoms based on the development for the calculation of multicenter integrals over noninteger n-STOs.

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