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Full Length Research Paper

Calculation of two-center overlap integrals over slater-type orbitals via fourier transform convolution theorem

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Formulas for two-center overlap integrals over slater type orbitals are presented. The established formula contains Gaunt coefficients and auxiliary functions. Analytical and recurrence relations for these auxiliary functions have been presented. The efficiency of the presented algorithm for the evaluation of two-center overlap integrals depends strictly on the accurate calculation of these auxiliary functions. It is shown that our algorithm agrees well with the available literature datas, for a wide range of quantum numbers, orbital exponents and internuclear distances.

Key words: Slater type orbital, overlap integral, Gaunt coefficient, auxilary function.

INTRODUCTİON

The most widely used method for constructing approximate molecular wave functions is linear combination of atomic orbitals (LCAO) (Roothaan, 1951) (Roothaan, 1960). The commonly used orbitals in literature are the Slater-type orbitals (STOs) (Slater, 1930; Zener, 1930) and Gaussian-type orbitals (GTOs) (Boys, 1950). A well behaved basis function must satisfy the Kato cusp condition near the nuclei and decay exponentially far from the nuclei (Kato, 1957; Agmon, 1982). As is well-known; while STOs satisfy the abovementioned criteria, GTOs do not. Since the calculation of molecular integrals over STOs is complex, their use in large scale electronic structure calculations was hindered in the middle of the past century. Then, a pragmatic solution proposed by Boys (1950) was the use of GTOs instead of STOs to overcome the computational difficulties of the multicenter integrals over STOs. This situation has been maintained up to 1980s and led to some popular electronic structure calculation programs such as GAUSSIAN. Due to the improvement in the applied mathematics and computer technology, nowadays, there are a renewed interest in the calculation of molecular integrals over STOs (Barnett, 2000a, b; 2002; 2003a, b, c; 1990; 1991; 1993; 2007; Barnett and Perry, 1994; Harris, 1960, 1997, 2002, 2007; Harris and Michels, 1965, 1966; 1967; Bouferguene and Rinaldi; 1994; Bouferguene et al., 1996; Jones, 1997; Bouferguene and Jones, 1998; Jain et al., 2004; Bouferguene, 2005; Weatherford et al., 2006; Absi and Hoggan, 2006; Duret et al., 2008; Hoggan, 2009; Safouhi, 2009; Steinborn and Filter, 1975; 1978; Trivedi annd Steinborn, 1983; Weniger and Steinborn, 1983, 1988; Weniger et al., 1986, Homeier and Steinborn, 1990, 1991, 1993; Steinborn et al., 1992, 2000; Maslov et al., 1995; Weniger, 2008; Rico et al., 1988, 1989, 1992, 1994, 1998, 2000a, b, 2010; Ema et al., 2008; Niehaus et al., 2008; Guseinov, 1970, 2004, 2005, 2010, 1985; Guseinov and Mamedov, 1999, 2000; Guseinov et al., 2000; Mamedov, 2004; Mamedov and Koç, 2008; Magnasco et al., 1998, 1999; Magnasco and Rapallo, 2000; Ozdogan and Orbay, 2002a, b; Ozdogan et al., 2002, 2003, 2005; Gümüş and Ozdogan, 2003; Ozdogan, 2003, 2004a, b, c, 2008; Gümüş and Ozdogan, 2004a, b; Hoggan et al., 2010; Oztekin et al., 2001, 2002; Oztekin, 2004; Yavuz et al., 2005; Oztekin and Ozcan, 2007; Transworld Research Network, 2008; Weniger, 2008a, b, c, d; Transworld Research Network, 2008).

The use of single-center expansion methods (Barnett and Coulson, 1951; Harris and Michels, 1966, 1967; Bouferguene and Rinaldi, 1994; Jones, 1997; Niehaus et al., 2008) enables one to express the three-center nuclear attraction and three- and four-center electron repulsion integrals in terms of two-center overlap

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integrals. Thus, two-center overlap integrals are regarded as basic building block of molecular integrals and therefore, their rapid and efficient calculation is of prime importance. Although there are several algorithms in the literature for the calculation of two-center overlap integrals over STOs (Barnett, 2000a, b; 2002; 2003a, b, c; 1990; 1991; 1993; 2007; Barnett and Perry, 1994; Harris, 1960, 1997, 2002, 2007; Harris and Michels, 1965, 1966; 1967; Bouferguene and Rinaldi; 1994; Bouferguene et al., 1996; Jones, 1997; Bouferguene and Jones, 1998; Jain et al., 2004; Bouferguene, 2005; Weatherford et al., 2006; Absi and Hoggan, 2006; Duret et al., 2008; Hoggan, 2009; Safouhi, 2009; Steinborn and Filter, 1975; 1978; Trivedi annd Steinborn, 1983; Weniger and Steinborn, 1983; Weniger et al., 1986, 1988, Homeier and Steinborn, 1990, 1991, 1993; Steinborn et al., 1992, 2000; Maslov et al., 1995; Weniger, 2008; Rico et al., 1988, 1989, 1992, 1994, 1998, 2000a, b, 2010; Ema et al., 2008; Niehaus et al., 2008; Guseinov, 1970, 2004, 2005, 2010, 1985; Guseinov and Mamedov, 1999, 2000; Guseinov et al., 2000; Mamedov, 2004; Mamedov and Koç, 2008; Magnasco et al., 1998, 1999; Magnasco and Rapallo, 2000; Ozdogan and Orbay, 2002a, b; Ozdogan et al., 2002, 2003, 2005; Gümüş and Ozdogan, 2003; Ozdogan, 2003, 2004a, b, c, 2008; Gümüş and Ozdogan, 2004a, b; Hoggan et al., 2010; Oztekin et al., 2001, 2002; Oztekin, 2004; Yavuz et al., 2005; Oztekin and Ozcan, 2007; E.J. Weniger, 2008a, b, c, d), it is well-known that some of these algorithms/formulas are complex in structure and suffer from some stability problems, especially for the cases below:

i large internuclear distances and different orbital exponents,
ii small internuclear distances and nearly equal orbital exponents,
iii equal orbital exponents.

To overcome the computational difficulties and instability problems, recently, we have reported analytical and recurrence formulae for the evaluation of two-center overlap integrals over STOs (Guseinov et al., 2000; Ozdogan and Orbay, 2002a, b; Ozdogan et al., 2002, 2003, 2005; Gümüş and Ozdogan, 2003; Ozdogan, 2003; Gümüş and Ozdogan, 2004a, b; Ozdogan, 2004a, b, c, 2008; Hoggan et al., 2010), using the elliptical coordinates method, translation methods, and the Fourier transform convolution theorem. The formula we presented with Fourier transform convolution theorem is the same as that presented by Ozdogan (2004a), was promising except for the infinite sums in the structure of the formula. The aim of this work is to provide an efficient and rapid analytical algorithm for the evaluation of two-center overlap integrals over STOs in general coordinate system (lined-up or nonlined-up) using Fourier transform convolution theorem, which does not seem to be affected from the stability problems mentioned above.

General definitions

The two-center overlap integrals over STOs examined in the present work have the following form

$$S_{nlm,n'l'm'}\left(\zeta,\zeta';\vec{R}\right)=\int\chi^{*}_{nlm}\left(\zeta,\vec{r}\right)\chi_{n'l'm'}\left(\zeta',\vec{r}-\vec{R}\right)d^{3}r, \quad (1)$$

where $\chi_{nlm}\left(\zeta,\vec{r}\right)$ and $\chi_{n'l'm'}\left(\zeta',\vec{r}-\vec{R}\right)$ are normalized real or complex STOs located on centers $\vec{r}$ and $\vec{r}-\vec{R}$, respectively. The STO is defined as

$$\chi_{nlm}\left(\zeta,\vec{r}\right)=N_{n}\left(\zeta\right)r^{n-1}e^{-\zeta r}S_{lm}\left(\theta,\varphi\right) \quad (2)$$

where ζ is orbital exponent, $N_{n}\left(\zeta\right)$ is normalization constant given by

$$N_{n}\left(\zeta\right)=\frac{\left(2\zeta\right)^{n+\frac{1}{2}}}{\sqrt{(2n)!}}, \quad (3)$$

and $S_{lm}\left(\theta,\varphi\right)$ is complex or real spherical harmonics defined by Abramowitz and Stegun (1965):

$$S_{lm}\left(\theta,\varphi\right)=\mathscr{P}_{lm}\left(cos\,\theta\right)\Phi_{m}\left(\varphi\right) \quad (4)$$

in which surface spherical harmonics $\Phi_{m}\left(\varphi\right)$ are defined.

For complex spherical harmonics:

$$\Phi_{m}\left(\varphi\right)=\frac{e^{im\varphi}}{\sqrt{2\pi}} \quad (5)$$

for real spherical harmonics:

$$\Phi_{m}\left(\varphi\right)=\frac{1}{\sqrt{\pi\left(1+\delta_{m0}\right)}}\begin{cases}cos\left(|m|\varphi\right)\ ; & \text{for } m\geq 0\\ sin\left(|m|\varphi\right)\ ; & \text{for } m<0\end{cases} \quad (6)$$

The function $\mathscr{P}_{lm}\left(cos\,\theta\right)$ in Equation (4) is normalized associate Legendre function (Abramowitz and Stegun, 1965).

Two-center overlap integrals over STOs

Following the Fourier transform convolution theorem, the two-center overlap integrals over STOs given by Equation (1) take the form:

$$S_{nlm,n'l'm'}\left(\zeta,\zeta';\vec{R}\right)=\int U^{*}_{nlm}\left(\zeta,\vec{p}\right)U_{n'l'm'}\left(\zeta',\vec{p}\right)e^{-i\vec{p}\vec{R}}d^{3}p \qquad (7)$$

where the functions $U_{nlm}\left(\zeta,\vec{p}\right)$ and $U_{n'l'm'}\left(\zeta',\vec{p}\right)$ are Fourier transforms of STOs, analytical and alternative formulas are presented in Appendix A.

For the calculation of two-center overlap integrals over real STOs, first we substitute the plane wave expansion by the term $e^{-i\vec{p}\vec{R}}$ (Gradshteyn and Ryzhik, 1995)

$$e^{-i\vec{p}\vec{R}}=4\pi\sum_{L=0}^{\infty}\left(-i\right)^{L}j_{L}\left(pR\right)\sum_{M=-L}^{L}S^{*}_{LM}\left(\hat{R}\right)S_{LM}\left(\hat{p}\right) \qquad (8)$$

and the mathematical formula for the Fourier transform of STOs given at Appendix A into Equation (7), then we obtain

$$S_{nlm,n'l'm'}\left(\zeta,\zeta';\vec{R}\right)=8N_{n}\left(\zeta\right)N_{n'}\left(\zeta'\right)\sum_{L=0}^{\infty}\left(-1\right)^{\frac{1}{2}\left(l+3l'+3L\right)}\sum_{M=-L}^{L}G^{LM}_{lm,l'm'}S_{LM}\left(\vec{R}\right)D^{2,L}_{n+1,l;n'+1,l'}\left(\zeta,\zeta';R\right) \qquad (9)$$

in Equation (8), the function $j_{n}\left(x\right)$ is spherical Bessel function (Gradshteyn and Ryzhik, 1995) and the function $G^{LM}_{lm,l'm'}$ in Equation (9) is defined according to Rico et al. (1988):

$$G^{LM}_{lm,l'm'}=\int_{\Omega_p}S^{*}_{lm}\left(\hat{p}\right)S_{l'm'}\left(\hat{p}\right)S_{LM}\left(\hat{p}\right)d\Omega_{p}=\sqrt{\frac{2L+1}{4\pi}}C^{L|M|}\left(lm,l'm'\right)A^{M}_{mm'} \qquad (10)$$

where the coefficients $C^{L|M|}\left(lm,l'm'\right)$ in Equation (10) are related to the Gaunt coefficients and given by

$$C^{L|M|}\left(lm,l'm'\right)=\sqrt{\frac{2}{2L+1}}\int_{0}^{\pi}\mathcal{P}_{lm}\left(\cos\theta\right)\mathcal{P}_{l'm'}\left(\cos\theta\right)\mathcal{P}_{LM}\left(\cos\theta\right)\sin\theta d\theta$$

$$=\begin{cases}C^{L}\left(lm;l'm'\right) & ;\ if\ \left|M\right|=\left|m-m'\right|\\ C^{L}\left(lm;l'-m'\right) & ;\ if\ \left|M\right|=\left|m+m'\right|\end{cases} \qquad (11)$$

in which $C^{L}\left(lm,l'm'\right)$ are the well-known Gaunt coefficients. Due to the properties of Gaunt cofficients, the values of L in Equation (9) are restricted and can take only the values in range below with step two

$$\left|l-l'\right|\le L\le\left(l+l'\right). \qquad (12)$$

The function $A^{M}_{mm'}$ in Equation (10) is defined by the following integral formula

$$A^{M}_{mm'}=\sqrt{2\pi}\int_{0}^{2\pi}\Phi^{*}_{m}\left(\varphi\right)\Phi_{m'}\left(\varphi\right)\Phi_{M}\left(\varphi\right)d\varphi \qquad (13)$$

and the analytical formula for the function $A^{M}_{mm'}$ can be found somewhere else (Guseinov, 1970) or can be calculated using Maple softwave for any special values of M, m and m'.

Taking into account the criteria given by Equaation (12) and substituting Equation (10) into Equation (9), we get the following compact formula for the two-center overlap integrals over real STOs:

$$S_{nlm,n'l'm'}\left(\zeta,\zeta';\vec{R}\right)=\sum_{L=\left|l-l'\right|}^{l+l'}{}^{(2)}\sum_{M=-L}^{L}H^{LM}_{nlm,n'l'm'}\left(\zeta,\zeta'\right)D^{2,L}_{n+1,l;n'+1,l'}\left(\zeta,\zeta';R\right)S_{LM}\left(\theta,\varphi\right) \qquad (14)$$

Here $S_{LM}\left(\theta,\varphi\right)$ stays for real spherical harmonics (Abramowitz and Stegun, 1965) and the function $H^{LM}_{nlm,n'l'm'}\left(\zeta,\zeta'\right)$ is defined by

$$H^{LM}_{nlm,n'l'm'}\left(\zeta,\zeta'\right)=\left(-1\right)^{\frac{1}{2}\left(l+3l'+3L\right)}4N_{n}\left(\zeta\right)N_{n'}\left(\zeta'\right)\sqrt{\frac{2L+1}{\pi}}C^{L|M|}\left(lm,l'm'\right)A^{M}_{mm'} \qquad (15)$$

and the symbol $\sum^{(2)}$ in Equation (14) indicates that the summation is performed in steps of two, which is related to the nonzero Gaunt coefficients. The auxiliary function $D^{2,L}_{nl;n'l'}(\zeta,\zeta';R)$ in Equation (14) is analysed.

Repeating the steps described above for the case of real STOs, the following analytical formula for the two-center overlap integrals over complex STOs can be obtained:

$$S_{nlm,n'l'm'}\left(\zeta,\zeta';\vec{R}\right)=\sum_{L=|l-l'|}^{l+l'}{}^{(2)}H^{L}_{nlm,n'l'm'}(\zeta,\zeta')D^{2,L}_{n+1,l;n'+1,l'}(\zeta,\zeta';R)Y_{L,m-m'}(\theta,\varphi) \qquad (16)$$

where $Y_{L,m-m'}(\theta,\varphi)$ are the complex spherical harmonics (Abramowitz and Stegun, 1965) and we define the function $H^{L}_{nlm,n'l'm'}(\zeta,\zeta')$ as

$$H^{L}_{nlm,n'l'm'}(\zeta,\zeta')=(-1)^{\frac{1}{2}(3L+3l'+l)}4N_n(\zeta)N_{n'}(\zeta')\sqrt{\frac{2L+1}{\pi}}C^{L}(lm,l'm')\delta_{mm'} \quad (17)$$

in which $\delta_{mm'}$ is well-known kronecker delta function (Abramowitz and Stegun, 1965).

The unified expression, Equation (14), we presented for two-center overlap integrals over STOs in nonlined-up coordinate systems reduces to a simple form in case of lined-up coordinate systems as follow:

$$S_{nlm,n'l'm}(\zeta,\zeta';R)=\sum_{L=|l-l'|}^{l+l'}{}^{(2)}\sqrt{\frac{2L+1}{4\pi}}H^{L0}_{nlm,n'l'm}(\zeta,\zeta')D^{2,L}_{n+1,l;n'+1,l'}(\zeta,\zeta';R) \quad (18)$$

and the auxiliary function $F^{mL}_{nn'}(\zeta,\zeta';R)$ will be defined in next sub-section and analysed in a detailed way.

Auxiliary functions

In this section, we provide more details of the analytical calculation of the auxiliary functions which appear in our algorithm.

Auxiliary function $D^{2,L}_{nl;n'l'}(\zeta,\zeta';R)$

The auxiliary function $D^{2,L}_{nl;n'l'}(\zeta,\zeta';R)$ which appear in Equations (9) and (14) is given by the following integral formula:

$$D^{2,L}_{nl;n'l'}(\zeta,\zeta';R)=\int_0^\infty p^2 D_{nl}(\zeta,p)D_{n'l'}(\zeta',p)j_L(pR)dp. \quad (19)$$

Using Equation (B.1) of Appendix B for the functions $D_{nl}(\zeta,p)$ and $D_{n'l'}(\zeta',p)$ in Equation (19) we get the relation below for the auxiliary function $D^{2,L}_{nl;n'l'}(\zeta,\zeta';R)$:

$$D^{2,L}_{n,l;n',l'}(\zeta,\zeta';R)=\sum_{s=0}^{E\left(\frac{n-l-1}{2}\right)}A^{s}_{nl}(\zeta)\sum_{s'=0}^{E\left(\frac{n'-l'-1}{2}\right)}A^{s'}_{n'l'}(\zeta')F^{l+l'+2s+2s'+2,L}_{nn'}(\zeta,\zeta';R). \quad (20)$$

Here, the symbol $E\left(\frac{n}{2}\right)$ means

$$E\left(\frac{n}{2}\right)=\frac{n}{2}-\frac{1}{4}\left[1-(-1)^n\right] \qquad (21)$$

Auxiliary function $F^{mL}_{nn'}(\zeta,\zeta';R)$

The auxiliary function $F^{mL}_{nn'}(\zeta,\zeta';R)$ is given by the following integral formula:

$$F^{mL}_{nn'}(\zeta,\zeta';R)=\int_0^\infty \frac{p^m}{\left(p^2+\zeta^2\right)^n\left(p^2+\zeta'^2\right)^{n'}}j_L(pR)dp \qquad (22)$$

Employing the relation from the literature (Weniger and Steinborn, 1983; Ozdogan, 2004a) for $\left(p^2+\zeta^2\right)^{-n}\left(p^2+\zeta'^2\right)^{-n'}$

$$\left(p^2+\zeta^2\right)^{-n}\left(p^2+\zeta'^2\right)^{-n'}=\sum_{i=0}^{n-1}\gamma^{i}_{nn'}(\zeta,\zeta')\left(p^2+\zeta^2\right)^{-i-1}+\sum_{j=0}^{n'-1}\gamma^{j}_{n'n}(\zeta',\zeta)\left(p^2+\zeta'^2\right)^{-j-1} \quad (23)$$

with

$$\gamma^{i}_{nn'}(\zeta,\zeta')=(-1)^{n'}F_{n'-1}(n+n'-i-2)\left(\zeta^2-\zeta'^2\right)^{i-(n+n')+1} \qquad (24)$$

in Equation (22), it is easy to obtain the following analytical formula for the auxiliary function $F^{mL}_{nn'}(\zeta,\zeta';R)$:

$$F_{n'}^{mL}(\zeta,\zeta';R)=\sum_{i=0}^{n-1}\gamma_{nn'}^{i}(\zeta,\zeta')E_{m,i+1}^{L}(\zeta,R)+\sum_{j=0}^{n'-1}\gamma_{n'n}^{j}(\zeta',\zeta)E_{m,j+1}^{L}(\zeta',R) \quad (25)$$

For the special case $\zeta=\zeta'$, Equation (25) reduces to the relation below:

$$F_{nn'}^{mL}(\zeta,\zeta;R)=E_{m,n+n'}^{L}(\zeta,R) \quad (26)$$

The auxiliary function $E_{mn}^{L}(\zeta,R)$ appearing in Equations (25) and (26) will be defined in next sub-section and analysed in a detailed way.

Auxiliary function $E_{mn}^{L}(\zeta,R)$

The auxiliary function $E_{mn}^{L}(\zeta,R)$ is given by the following integral formula

$$E_{mn}^{L}(\zeta,R)=\int_0^{\infty}\frac{p^m}{(p^2+\zeta^2)^n}j_L(pR)dp \quad (27)$$

Here $j_L(x)$ are spherical Bessel functions (Gradshteyn and Ryzhik, 1995). Spherical Bessel functions can be described in terms of sinus and cosinus functions as presented by Monserrat and Haynes (2010).

$$j_L(x)=\sum_{k=0}^{E\left(\frac{L}{2}\right)}\frac{A_{Lk}\sin\left(x-\frac{L\pi}{2}\right)}{x^{2k+1}}+\sum_{k'=0}^{E\left(\frac{L-1}{2}\right)}\frac{B_{Lk'}\cos\left(x-\frac{L\pi}{2}\right)}{x^{2k'+2}} \quad (28)$$

where the coefficients A_{Lk} and B_{Lk} are defined as follow:

$$A_{Lk}=\frac{(-1)^k(2k)!}{2^{2k}}F_{2k}(L+2k)F_{2k}(L) \quad (29.a)$$

$$B_{Lk}=\frac{(-1)^k(2k+1)!}{2^{2k+1}}F_{2k+1}(L+2k+1)F_{2k+1}(L) \quad (29.b)$$

Substituting Equations (28) and (29) in Equation (27), we get the compact formula for the auxiliary function $E_{mn}^{L}(\zeta,R)$

$$E_{mn}^{L}(\zeta,R)=\sum_{k=0}^{E\left(\frac{L}{2}\right)}\frac{A_{Lk}}{R^{2k+1}}(-1)^{F\left(\frac{L}{2}\right)}G_{m-2k-1,n}(\zeta,R)+\sum_{k'=0}^{E\left(\frac{L-1}{2}\right)}\frac{B_{Lk'}}{R^{2k'+2}}(-1)^{E\left(\frac{L}{2}\right)}G_{m-2k-2,n}(\zeta,R) \quad (30)$$

Here, the symbol $F\left(\frac{n}{2}\right)$ means

$$F\left(\frac{n}{2}\right)=\frac{n}{2}+\frac{1}{4}\left[1-(-1)^n\right] \quad (31)$$

and the auxiliary function $G_{mn}(\zeta,R)$ is defined as:

$$G_{mn}(\zeta,R)=\begin{cases}J_{mn}(\zeta,R) & ;\ \text{if } m \text{ even}\\ I_{mn}(\zeta,R) & ;\ \text{if } m \text{ odd}\end{cases} \quad (32)$$

Here the functions $I_{mn}(\zeta,R)$ and $J_{mn}(\zeta,R)$ are investigated in detail in Appendix B.

In order to have an alternative formula for the auxiliary function $E_{mn}^{L}(\zeta,R)$ we employ Equation (A.13) in Equation (27) and then we get

$$E_{mn}^{l}(\zeta,R)=\sum_{k=1}^{l}a_{lk}(-1)^{1-k}\sum_{s=0}^{l-k+1}(-1)^{F\left(\frac{s}{2}\right)}\frac{(l-k+1)!}{s!\,R^{l-s+1}}\left[\eta_s^{-}J_{m-l+s-1,n}(\zeta,R)+\eta_s^{+}I_{m-l+s-1,n}(\zeta,R)\right]. \quad (33)$$

Utilizing the recurrence relation for spherical Bessel function (Gradshteyn and Ryzhik, 1995)

$$j_{l+1}(x)=\frac{2l+1}{x}j_l(x)-j_{l-1}(x) \quad (34)$$

in Equation (27), it is easy to obtain recurrence formulae for the auxiliary function $E_{mn}^{l}\left(\zeta,R\right)$ by

$$E_{mn}^{l+1}\left(\zeta,R\right)=\frac{2l+1}{R}E_{m-1,n}^{l}\left(\zeta,R\right)-E_{mn}^{l-1}\left(\zeta,R\right) \quad (35.a)$$

$$E_{mn}^{L}\left(\zeta,R\right)=E_{m-2,n-1}^{L}\left(\zeta,R\right)-\zeta^{2}E_{m-2,n}^{L}\left(\zeta,R\right) \quad (35.b)$$

with the starting values

$$E_{mn}^{0}\left(\zeta,R\right)=R^{-1}I_{m-1,n}\left(\zeta,R\right) \quad (36.a)$$

$$E_{mn}^{1}\left(\zeta,R\right)=R^{-2}I_{m-2,n}\left(\zeta,R\right)-R^{-1}J_{m-1,n}\left(\zeta,R\right) \quad (36.b)$$

Since these starting values are calculated analytically, the use of the recurrence relations does not cause digital erosion in the calculations, and therefore these recursion relations are stable.

COMPUTATIONAL RESULTS AND DISCUSSION

In this work we have presented an analytical algorithm for the evaluation of the two-center overlap integrals in a general coordinate system using the Fourier transform convolution theorem. Our algorithm involves the calculation of Gaunt coefficients, auxiliary functions $D_{nl;n'l'}^{2,L}\left(\zeta,\zeta';R\right)$ and spherical harmonics. The obtained formula for the two-center overlap integrals over STOs is valid for the cases of lined-up and nonlined-up coordinate systems. Higher accuracy in the calculation of two-center overlap integrals over STOs depends strickly on the accurate calculation of the auxiliary function $D_{nl;n'l'}^{2,L}\left(\zeta,\zeta';R\right)$. Therefore, we have focused our attention on the accurate calculation of this auxiliary function by introducing analytic recursive and alternative formulae for the auxiliary functions appearing in the calculations.

We have written computer programs in Maple 13 symbolic programming language (Maple 13) for the evaluation of two-center overlap integrals over STOs based on Equation (14). In order to illustrate the efficiency of our algorithm, we have performed an extensive study in which quantum numbers, orbital exponents and locations of STOs vary over wide ranges. Our computational results of two-center overlap integrals over STOs have been compared with the ones available of the literatüre and can be seen in Table 1.

As can be seen in Table 1 that our computer results for two-center overlap integrals are in best agreement with avaliable literature values (Barnett, 2002; 2003a; Safouhi, 2009; Guseinov and Mamedov, 1999; Mamedov and Koç, 2008; Guseinov and Mamedov, 2000; Mamedov, 2004; Magnasco et al., 1999; Ozdogan, 2004a, b; Yavuz et al., 2005; Romanowski and Jalbout, 2009) except for the intgerals we have labeled with 15, 23, 35, 36 and 43. The literature values for the integrals 15, 23, 35, 36 and 43 are presented by Mamedov (2004), Gümüş and Ozdogan (2004a), Mamedov and Koç (2008), Barnett (2007) and Ozdogan (2004a), respectively. Looking back to the programs we presented by Ozdogan (2004a), we see that the integral values we can observe with 23 and 43 are erroneous and we conclude that these values have been missprinted. Using the presented procedure and our previous procedures (Ozdogan et al., 2002, 2005), we could not get the literature value for the integral we labeled with 15, 35 and 36. The integral we labeled with 36 is in lined-up coordinate system. For this integral, we have used our general formula given by Equation (14), our simplified formula given by Equation (18) and our previous algorithms, but we could not get the literature value for the integral 36. The integral we labeled with 15 and 35 is in nonlined-up coordinate system. The available literature by Mamedov and Koç (2008) and Mamedov (2004) for these integrals use the rotation of two-center overlap integrals in lined-up coordinate system. That means in this references and also in our previous paper (Ozdogan et al., 2002, 2005), two-center overlap integrals are expressed in terms of rotation coefficients of two-center overlap integrals in lined-up coordinate systems and two-center overlap integrals in lined-up coordinate systems. Despite the fact that we use the computer programs with the same method that was used by Mamedov and Koç, (2008) and Mamedov (2004), we were not able to get the compatible values for the integrals 15 and 35. On the other hand, we get exactly the same results from our procedure here. Therefore, these integrals might have been missprinted or are erroneous.

The computational time for the calculation of two-center overlap integrals over STOs are long due to the Maple programming language. This programming language has been used to test the accuracy of our algorithm. The accuracy and speed of our algorithm depend on the accurate and the speed calculation of the auxiliary function $D_{nl;n'l'}^{2,L}\left(\zeta,\zeta';R\right)$. Therefore, by storing this auxiliary function into a one dimensional array in the memory of the computer during the compilation of the program and getting back from the memory during the calculation will reduce the computational time drastically. It is possible to write a fast computer program in Fortran language that use the idea above.

As a conclusion, we conclude that the procedure we presented here enable one can add fast, accurate and stable calculation of two-center overlap integrals over STOs in which quantum numbers, orbital exponents and internuclear distances were varied over wide ranges. In view of the accuracy and speed of the presented algorithm for two-center overlap integrals over STOs, we anticipate that our algorithm can prove to be of great

Table 1. The comparative values of two-center overlap integrals over real STOs*.

Nu	n	l	m	n'	l'	m'	ξ	ξ'	R	θ	φ	This work – Equation (14)	Literature	Reference
1	1	0	0	1	0	0	5.8	4.2	0.5	30	135	0.450 897 002 422 256×10^{0}		
2	1	0	0	2	1	0	1.3	2.3	0.2	0	0	0.143 974 188 820 009×10^{0}	0.143 974 188 822×10^{0}	Magnasco et al. (1999)
3	1	0	0	2	1	0	10	2	1.4	0	0	0.117 413 789 686 628×10^{0}	-0.117 413 789 68 662 828 485 49×10^{0}	Barnett (2003a)
4	2	0	0	2	0	0	2	4	5	30	60	0.214 404 132 575 179×10^{-2}		
5	2	1	0	5	2	0	2	0.3	1.4	0	0	-0.233 230 081 719 942×10^{-2}	-0.233 230 081 719 942989 706×10^{-2}	Barnett (2003a)
6	2	1	1	2	1	0	11.9	3.6	5	40	180	-0.269 946 219 027 026×10^{-6}	-0.269 946 218 955 806×10^{-6}	Mamedov (2004)
7	2	1	0	3	2	0	0.6	5.1	2.5	0	0	0.158 946 116 138 954×10^{-2}	0.158 946 116 139×10^{-2}	Magnasco et al. (1999)
8	2	1	1	2	0	0	7.5	5	6	60	45	0.462 084 402 132 043×10^{-10}		
9	2	1	-1	2	1	-1	2.4	4.1	2.5	0	0	-0.254 205 622 595 321×10^{-1}	0.254 205 622 595×10^{-1}	Magnasco et al. (1999)
10	3	2	0	3	2	0	7.5	2.5	5	60	120	-0.680 340 033 602 071×10^{-4}	-0.680 340 033 108 123×10^{-4}	Ozdogan (2004a)
11	3	2	0	5	2	0	1.5	0.3	1.4	0	0	0.122 836 359 643 126×10^{-1}	0.122 836 359 643 126 249 448×10^{-1}	Barnett (2003a)
12	3	2	1	3	2	1	6.5	2	1.4	0	0	0.959 577 534 408 839×10^{-1}	0.959 577 534 408 839 815 43×10^{-1}	Ozdogan (2004b)
13	3	2	1	2	1	-1	6	2	4	30	60	-0.109 274 543 457 121×10^{-2}	-0.109 274 543 461 435×10^{-2}	Yavuz et al. (2005)
14	3	2	1	3	2	1	7	3	5	0	0	-0.442 287 766 988 256×10^{-4}	-0.442 287 766 988 261×10^{-4}	
15	3	2	1	2	1	1	7	4	3	120	90	-0.153 446 035 282 096×10^{-3}	-0.850 274 361 752 408×10^{-5}	Mamedov (2004)
16	3	2	1	3	2	0	9.7	6.4	0.3	20	135	0.137 350 765 843 157×10^{-1}	-0.137 350 765 807 479×10^{-1}	Mamedov (2004)
17	3	2	2	3	2	2	5.8	5.8	0.2	0	0	0.909 920 806 903 332×10^{0}	0.909 920 806 903 332×10^{0}	Yavuz et al. (2005)
18	3	2	0	3	2	0	2.3	5.1	8.7	0	0	0.323 123 695 513 570×10^{-5}	0.323 123 695 508×10^{-5}	Magnasco et al. (1999)
19	4	0	0	4	1	0	1.5	0.3	1.4	0	0	0.476 529 568 265 699×10^{-1}	-0.476 529 568 265 699 140 022×10^{-1}	Barnett (2003a)
20	4	3	3	4	2	2	10.8	6.1	1.2	120	360	0.233 631 800 354 459×10^{-1}	-0.233 631 800 354 459×10^{-1}	Mamedov (2004)
21	4	2	1	4	3	1	7	3	16	0	0	0.403 505 950 326 822×10^{-16}	0.403 505 950 326 822 9×10^{-16}	Barnett (2002)
22	4	3	0	4	3	2	7.5	2.5	30	60	30	-0.682 374 169 304 497×10^{-28}		
23	4	3	3	4	3	2	3	2	20	30	60	0.139 582 818 809 152×10^{-12}	0.375 545 611 854 747×10^{-1}	Ozdogan (2004a)
24	5	0	0	5	0	0	0.1	0.1	1.4	0	0	0.999 637 189 410 385×10^{0}	0.999 637 189 410 385 856 139 3×10^{0}	Ozdogan (2004b)
25	5	4	0	5	4	0	0.1	0.1	1	0	0	0.997 469 850 695 778×10^{0}	0.997 469 850 7×10^{0}	Romanowski and Jalbout (2009)
26	5	4	2	5	4	0	17	3	10	45	210	-0.134 568 733 968 070×10^{-10}	-0.134 568 733 674 016×10^{-10}	Yavuz et al. 2005
27	5	4	2	5	4	0	8.5	1.5	30	45	210	-0.227 511 176 683 283×10^{-16}	-0.227 511 176 683 183×10^{-16}	Mamedov and Koç (2008)
28	5	4	4	5	4	4	5	0.1	1	0	0	0.729 455 903 527 048×10^{-6}	0.729 455 903 5×10^{-6}	Romanowski and Jalbout (2009)
29	5	3	-3	12	3	3	3	1	5	20	22.5	-0.727 184 863 851 718×10^{-7}	-0.727 184 864 173 319×10^{-7}	Yavuz et al. (2005)
30	6	3	2	8	5	2	1.4	0.6	40	0	0	-0.312 391 598 542 938×10^{-4}	-0.321 391 598 543 043×10^{-4}	Safouhi (2009)
31	6	3	2	5	2	2	4.8	4.8	2.5	180	60	-0.889 717 464 593 021×10^{-1}	-0.889 717 464 593 021×10^{-1}	Mamedov (2004
32	6	2	1	5	2	1	7.4	1.4	0.1	45	80	0.517 527 643 277 711×10^{-1}	0.517 325 355 481 882×10^{-1}	Mamedov (2004)
33	6	4	2	5	3	3	3.7	6.1	0.6	30	100	0.182 881 883 670 195×10^{-1}	-0.182 881 883 670 196×10^{-1}	Mamedov (2004)
34	7	3	2	4	3	2	8.5	1.5	30	0	0	0.176 861 050 692 264×10^{-17}	-0.176 861 050 692 264×10^{-17}	Barnett (2002)
35	7	4	1	5	3	1	8.5	1.5	40	45	210	0.646 179 943 324 138×10^{-23}	-0.200 183 868 910 395×10^{-22}	Mamedov and Koç (2008)

Table 1. Contd.

36	7	4	4	7	4	4	4	3	1	0	0	0.651 867 026 918 169$\times10^{0}$	0.110 110 477 764 970 217$\times10^{0}$	Barnett (2003a)
37	8	0	0	8	0	0	5	1	1	0	0	0.107 437 341 693 226$\times10^{0}$	0.107 437 341 7$\times10^{0}$	Romanowski and Jalbout (2009)
38	8	0	0	8	0	0	5	5	1	0	0	0.785 230 850 010 807$\times10^{0}$	0.785 230 850 0$\times10^{0}$	Romanowski and Jalbout (2009)
39	8	3	2	5	4	2	6	4	5	0	0	0.103 631 620 689 278$\times10^{-2}$		
40	8	3	2	6	5	4	8	2	5	30	120	0.411 170 867 232 093$\times10^{-5}$		
41	8	7	0	8	7	0	7	3	1	0	0	-0.480 476 832 860 554$\times10^{-1}$	-0.480 476 431 898 433$\times10^{-1}$	Guseinov and Mamedov (1999)
42	8	7	7	8	7	7	7	3	1	0	0	-0.126 219 198 648 448$\times10^{0}$	0.126 219 198 639 683$\times10^{0}$	Guseinov and Mamedov (1999)
43	8	7	-6	7	5	5	0.5	0.3	12	150	240	0.115 791 967 786 329$\times10^{0}$	-0.444 987 258 245 886$\times10^{-1}$	Ozdogan (2004a)
44	9	5	3	8	4	3	6	4	9	0	0	-0.546 510 243 022 704$\times10^{-7}$	-0.546 510 243 022 704$\times10^{-7}$	Barnett (2002)
45	9	3	1	7	4	0	6.5	3.5	10	45	150	-0.212 856 280 570 926$\times10^{-6}$		
46	10	0	0	10	0	0	8	2.5	3	0	0	0.219 689 181 056 372$\times10^{0}$	0.219 686 181 056 372 382$\times10^{0}$	Barnett (2003a)
47	10	7	1	8	1	1	2.5	2.5	10	0	0	0.152 138 456 890 819$\times10^{-1}$	0.152 138 456 890 817$\times10^{-1}$	Safouhi (2009)
48	10	7	1	8	2	1	6	4	12	0	0	-0.184 189 026 173 198$\times10^{-9}$	-0.184 189 026 173 198$\times10^{-9}$	Barnett (2002)
49	10	9	9	10	9	9	8	2	3	0	0	0.623 122 318 191 124$\times10^{-3}$	0.623 122 318 191 124$\times10^{-3}$	Mamedov and Koç (2008)
50	10	9	8	12	10	8	7	3	4	30	360	0.150 981 944 333 770$\times10^{-2}$	0.150 981 944 685 389$\times10^{-2}$	Guseinov and Mamedov (2000)
51	11	0	0	10	9	8	3.5	6.5	10	135	150	-0.398 814 402 495 692$\times10^{-7}$		
52	12	7	3	12	7	3	1.3	0.7	15	0	0	-0.229 354 175 182 345$\times10^{-1}$	-0.229 354 178 100 624$\times10^{-1}$	Safouhi (2009)
53	17	8	4	14	6	4	1.8	0.2	30	0	0	0.913 905 854 064 307$\times10^{-6}$	0.913 905 848 808 478$\times10^{-6}$	Safouhi (2009)
54	20	15	10	10	9	8	8.5	1.5	10	135	120	-0.539 872 139 429 768$\times10^{-12}$		
55	21	10	6	9	8	6	9	9	5	0	0	0.538 980 685 338 144$\times10^{-4}$	0.538 980 685 338 283$\times10^{-4}$	Safouhi (2009)
56	30	10	8	14	10	8	7	7	5	0	0	0.135 074 709 593 243$\times10^{-1}$	0.135 074 709 591 440$\times10^{-1}$	Safouhi (2009)
57	35	10	7	5	4	2	7.5	2.5	55	60	135	0.182 565 757 281 500$\times10^{-14}$		
58	38	10	8	30	10	8	8.5	1.5	4	0	0	0.136 385 841 503 310$\times10^{-5}$	0.136 385 965 917 645$\times10^{-5}$	Guseinov and Mamedov (2000)
59	40	4	3	12	4	3	4.8	1.2	5	0	0	0.948 379 220 832 556$\times10^{-1}$	0.948 359 636 822 715$\times10^{-1}$	Safouhi 2009
60	40	8	7	30	7	7	9.5	0.5	6	0	0	-0.470 039 545 615 360$\times10^{-16}$	-0.470 039 545 616 601$\times10^{-16}$	Guseinov and Mamedov (2000)
61	43	10	6	18	8	6	7.2	16.8	5	0	0	-0.115 825 653 267 175$\times10^{-3}$	-0.115 825 616 305 187$\times10^{-3}$	Guseinov and Mamedov (2000)
62	50	18	17	50	20	20	5.5	4.5	2	0	0	0.339 262 020 222 383$\times10^{0}$		
63	50	0	0	45	10	10	7.5	2.5	5	60	90	-0.156 344 305 010$\times10^{-5}$		

* The blancks in the right columns indicate that there are not available literature values.

value for large scale electronic structure calculation programs.

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APPENDIX

A. Fourier transforms of STOs

It is well-known that Fourier transform of any STO is written as follow:

$$U_{nlm}(\zeta,\vec{p}) = (2\pi)^{-3/2} \int \chi_{nlm}(\zeta,\vec{r}) e^{-i\vec{p}\vec{r}} d^3 r. \quad \text{(A.1)}$$

Substituting the definition of STOs in position space given by Equation (2) and plane wave expansion (Transworld Research Network, 2008; Guseinov et al. 2000; Ozdogan and Orbay, 2002a; Ozdogan and Orbay, 2002b; Ozdogan et al. 2002; Ozdogan et al. 2003; Gümüş and Ozdogan, 2003; Ozdogan, 2003; Gümüş and Ozdogan, 2004a; Ozdogan, 2004a; Ozdogan, 2004b; Ozdogan, 2004c; Gümüş and Ozdogan, 2004; Ozdogan et al. 2005; Ozdogan, 2008; Hoggan et al. 2010) given by Equation (8) for $e^{-i\vec{p}\vec{r}}$ into Equation (A.1), we get the relation

$$U_{nlm}(\zeta,\vec{p}) = \sqrt{\frac{2}{\pi}} N_n(\zeta) \sum_{L=0}^{\infty} \sum_{M=-L}^{L} (-i)^L S_{LM}(\hat{p}) \int_{k=0}^{\infty} r^{n+1} e^{-\zeta r} j_l(pr)\, dr \int_{\Omega_r} S_{lm}^*(\hat{r}) S_{LM}(\hat{r})\, d\Omega_r \quad \text{(A.2)}$$

Using the orhonormality of the spherical harmonics

$$\int_{\Omega_r} S_{lm}^*(\hat{r}) S_{LM}(\hat{r})\, d\Omega_r = \delta_{lL}\delta_{mM} \quad \text{(A.3)}$$

Equation (A.2) takes the form

$$\begin{aligned} U_{nlm}(\zeta,\vec{p}) &= (-i)^l \sqrt{\frac{2}{\pi}} N_n(\zeta) D_{n+1,l}(\zeta,p) S_{lm}(\theta,\varphi). \\ &= (-i)^l f_{nl}(\zeta,p) S_{lm}(\theta,\varphi) \end{aligned} \quad \text{(A.4)}$$

Here the function $D_{nl}(\zeta,p)$ is the integral of the form (Geller, 1963)

$$D_{nl}(\zeta,p) = \int_0^{\infty} r^n e^{-\zeta r} j_l(pr)\, dr \quad \text{(A.5)}$$

in which $j_l(x)$ is spherical Bessel function (Gradshteyn and Ryzhik, 1995).

The auxiliary functions $D_{nl}(\zeta,p)$ and $f_{nl}(\zeta,p)$ in Equation (A.4) are given by the following analytical formulae (Geller, 1963):

$$D_{nl}(\zeta,p) = \frac{1}{(p^2+\zeta^2)^n} \sum_{s=0}^{E\left(\frac{n-l-1}{2}\right)} A_{nl}^s(\zeta) p^{l+2s} \quad \text{(A.6)}$$

$$f_{nl}(\zeta,p) = \frac{1}{(p^2+\zeta^2)^n} \sum_{s=0}^{E\left(\frac{n-l}{2}\right)} B_{nl}^s(\zeta) p^{l+2s} \quad \text{(A.7)}$$

where the symbols $A_{nl}^s(\zeta)$ and $B_{nl}^s(\zeta)$ are

$$A_{nl}^s(\zeta) = (-1)^s 2^{2l+2s-n+1} (2\zeta)^{n-l-2s-1} (n-l-1)!\, l!\, F_{2l+2s+1}(n+l) F_s(l+s) \quad \text{(A.8)}$$

$$B_{nl}^s(\zeta) = \frac{(-1)^s}{\sqrt{\pi}} 2^{n+l+1} \zeta^{2n-l-2s+\frac{1}{2}} \frac{F_{2l+2s+1}(n+l+1) F_s(l+s)}{\sqrt{F_l(2l) F_{n-l}(2l) F_{n-l}(n+l)}} \quad \text{(A.9)}$$

To derive an alternative formula for the auxiliary function $D_{nl}(\zeta,p)$, first of all, we use the following relation for spherical Bessel function in terms of derivatives of zero-th order spherical Bessel function $j_0(x)$:

$$j_n(x) = (-x)^n \left(\frac{1}{x}\frac{d}{dx}\right)^n j_0(x) = (-1)^n \sum_{k=1}^{n} a_{nk} \frac{j_0^{(n-k+1)}(x)}{x^{k-1}} \quad \text{for } n \geq 1. \quad \text{(A.10)}$$

Here, the spherical Bessel function $j_0(x)$ is defined by Gradshteyn and Ryzhik (1995) as

$$j_0(x) = \frac{\sin x}{x} \quad \text{(A.11)}$$

and we define the coefficients a_{nk} by the following recurrence relation

$$a_{nk} = -(n+k-3) a_{n-1,k-1} + a_{n-1,k} \text{ for } (k \leq n) \quad \text{(A.12)}$$

with the starting value

Now, using the Leibnitz rule (Gradshteyn and Ryzhik, 1995) it is easy to obtain the relation below for *n*-th order derivatives of spherical Bessel function $j_0(x)$ as it follows

$$\frac{d^n}{dx^n} j_0(x) = \sum_{s=0}^{n} \frac{n!}{s!}\left[(-1)^{n+\frac{1}{2}\left(s+\eta_s^-\right)} \eta_s^- \frac{\cos x}{x^{n-s+1}} + (-1)^{n+\frac{1}{2}\left(s+\eta_s^-\right)} \eta_s^+ \frac{\sin x}{x^{n-s+1}} \right] \quad \text{(A.14)}$$

in which the symbols $\eta_s^{\pm}$ are

$$\eta_s^{\pm} = \frac{1}{2}\left[1 \pm (-1)^s\right]. \quad \text{(A.15)}$$

Substituting Equation (A.14) in (A.10), we get the following formula for spherical Bessel function $j_n(x)$ in terms of $sin(x)$ and $cos(x)$

$$j_n(x) = \sum_{k=1}^{n} a_{nk} (-1)^{k-1} \sum_{s=0}^{n-k+1} (-1)^{F\left(\frac{s}{2}\right)} \frac{(n-k+1)!}{s!}\left\{ \eta_s^- \frac{cos(x)}{x^{n-s+1}} + \eta_s^+ \frac{sin(x)}{x^{n-s+1}} \right\} \quad \text{(A.16)}$$

The use of Equation (A.16) in Equation (A.5), enables one to obtain the following expression for the auxiliary function $D_{nl}(\zeta, p)$

$$D_{nl}(\zeta,p) = \sum_{k=1}^{l} (-1)^{k-1} a_{lk} \sum_{s=0}^{l-k+1} (-1)^{\frac{1}{2}\left(s+\eta_s^-\right)} \frac{(l-k+1)!}{s!} p^{s-l-1}\left[\eta_s^- C_{n-l+s-1}(\zeta,p) + \eta_s^+ S_{n-l+s-1}(\zeta,p)\right] \quad \text{(A.17)}$$

In Equation (A.17), the functions $C_n(\zeta, p)$ and $S_n(\zeta, p)$ are defined by the following integral formulae

$$C_n(\zeta,p) = \int_0^{\infty} x^n e^{-\zeta x} cos(px)\, dx \quad \text{(A.18)}$$

$$S_n(\zeta,p) = \int_0^{\infty} x^n e^{-\zeta x} sin(px)\, dx \quad \text{(A.19)}$$

Analytical formulae for these integrals can be found elsewhere (Gradshteyn and Ryzhik, 1995). Employing the residue theorem to Equations (A.18) and (A.19), general formulae $C_n(\zeta, p)$ and $S_n(\zeta, p)$ can be found as in the following:

$$a_{n1} = 1. \quad \text{(A.13)}$$

$$C_n(\zeta,p) = \frac{n!}{\left(p^2+\zeta^2\right)^{n+1}} \sum_{k=\frac{1}{2}\left[1-(-1)^n\right]}^{n+1}{}^{(2)} (-1)^{E\left(\frac{k}{2}\right)} F_k(n+1)\, \zeta^{n-k+1} p^k, \quad \text{(A.20)}$$

$$S_n(\zeta,p) = \frac{n!}{\left(p^2+\zeta^2\right)^{n+1}} \sum_{k=1}^{n+1}{}^{(2)} (-1)^{\frac{k-1}{2}} F_k(n+1)\, \zeta^{n-k+1} p^k. \quad \text{(A.21)}$$

Here, the symbol $\sum^{(2)}$ in Equations (A.20) and (A.21) indicates that the summation proceeds in steps of two. Some analytical formulae for special cases of the functions $C_n(\zeta, p)$ and $S_n(\zeta, p)$ can be found elsewhere (Gradshteyn and Ryzhik, 1995). The formulae we presented above are general expressions and include less terms than others from the literature. Therefore there will be less computations during the calculation of the two-center overlap integrals over STOs.

B. Auxiliary Functions $I_{mn}(\zeta, R)$ and $J_{mn}(\zeta, R)$

C. The auxiliary functions $I_{mn}(\zeta, R)$ and $J_{mn}(\zeta, R)$ are integrals given by

$$I_{mn}(\zeta,R) = \int_0^{\infty} \frac{x^m}{\left(x^2+\zeta^2\right)^n} sin(Rx)\, dx; \quad \text{for odd } m \quad \text{(B.1)}$$

And

$$J_{mn}(\zeta,R) = \int_0^{\infty} \frac{x^m}{\left(x^2+\zeta^2\right)^n} cos(Rx)\, dx; \text{for even } m \quad \text{(B.2)}$$

The auxiliary functions $I_{mn}(\zeta, R)$ and $J_{mn}(\zeta, R)$ are defined with the condition $m \le 2n$. Some analytical and recurrence formulae for the simplified case of these auxiliary functions can be found elsewhere (Gradshteyn and Ryzhik, 1995). Utilizing the residue theorem in Equations (B.1) and (B.2), one can obtain easiliy the following analytical formulae for these auxiliary functions:

$$I_{mn}(\zeta,R)=\pi e^{-\zeta R}\sum_{k=0}^{min(n-1,2n-2)}F_{n-k-1}(2n-k-2)\sum_{s=0}^{k}(-1)^{\frac{3m+1}{2}-s}\frac{F_s(m)}{2^{m-s}}\frac{(2\zeta)^{k-s+m-2n+1}R^{k-s}}{(k-s)!}, \tag{B.3}$$

and

$$J_{mn}(\zeta,R)=\pi e^{-\zeta R}\sum_{k=0}^{min(n-1,2n-2)}F_{n-k-1}(2n-k-2)\sum_{s=0}^{min(k,m)}(-1)^{\frac{m}{2}-s}F_s(m)\frac{(2\zeta)^{k-s+m-2n+1}R^{k-s}}{2^{m-s}(k-s)!} \tag{B.4}$$

Recurrence relations for these auxiliary functions can be easily obtained as

$$I_{mn}(\zeta,R)=I_{m-2,n-1}(\zeta,R)-\zeta^2 I_{m-2,n}(\zeta,R) \tag{B.5}$$

$$J_{mn}(\zeta,R)=J_{m-2,n-1}(\zeta,R)-\zeta^2 J_{m-2,n}(\zeta,R) \tag{B.6}$$

The starting values in the recurrence relations above are obtained by

$$I_{-1,0}(\zeta,R)=\frac{\pi}{2}, \tag{B.7}$$

$$I_{-1,n}(\zeta,R)=\frac{\pi}{2\zeta^{2n}}\left[1-e^{-\zeta R}\sum_{k=0}^{n-1}\frac{F_k(n+k-1)}{2^{n+k-1}}\sum_{s=0}^{n-k-1}\frac{(\zeta R)^{n-k-s-1}}{(n-k-s-1)!}\right] \tag{B.8}$$

$$J_{0n}(\zeta,R)=\frac{\pi e^{-\zeta R}}{(2\zeta)^{2n-1}(n-1)!}\sum_{k=0}^{min(n-1,2n-2)}\frac{(2n-k-2)!}{(n-k-1)!k!}(2\zeta R)^k \tag{B.9}$$

These can be easily obtained by the use of the residue theorem.