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Non-Integer Slater Orbital Calculations
II. Two-Center Molecular Integrals

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In order to calculate the one- and two-electron, two-center integrals over non-integer n Slater type orbitals, use is made of elliptical coordinates for the monoelectronic, hybrid, and Coulomb integrals. For the exchange integrals, the atomic orbitals are translated to a common center. The final integration is performed by Gaussian quadrature.

As an example, an SCF *ab initio* calculation is performed for the LiH molecule, both with integer and non-integer principal quantum number.

Key words: Non-integer Slater integrals

1. Introduction

The Slater orbitals with non-integer n [1] provide a simple but more flexible basis for molecular calculations than the classical STOs. In the previous works, only monocentric calculations were carried out with non-integer STO (NISTO) [2, 3], excepting the work of M. Geller on the hydrogen-molecule ion. More recently, H. J. Silverstone [4] evaluated the two-center overlap and the Coulomb integrals using the Fourier transform convolution theorem, but his results are not very well adapted to practical use.

The purpose of this work is to evaluate all the diatomic molecular integrals. We use a Gaussian quadrature for the final integration.

2. Notations

$Y_{lm}(\Omega)$, spherical harmonics.

$\Gamma(\alpha)$, gamma function.

$\gamma(\alpha, x)$ and $\Gamma(\alpha, x)$ incomplete gamma functions.

$\mathscr{C}^{m_1 m_2 m_3}_{l_1 l_2 l_3} = C^{m_1 m_2 m_3}_{l_1 l_2 l_3} \times C^{0\,0\,0}_{l_1 l_2 l_3}$ product of Clebsch-Gordan coefficients.

$\mathscr{P}_{lm}(z)$ (resp. $P_{lm}(z)$) normed (resp. unnormed) Legendre polynomials also written $\mathscr{P}_{lm}(\xi, \eta)$ (resp. $P_{lm}(\xi, \eta)$) in ellipsoidal coordinates.

$\omega(\xi, \eta) = \xi + \eta + 1$.

$$N_{n\zeta} = \left[\frac{(2\zeta)^{2n+1}}{\Gamma(2n+1)}\right]^{1/2}$$ norm of the NISTO.

3. Choice of the Coordinate Systems

The following coordinate systems are used

1. Cartesian coordinates centered on the nuclei A and B. The z_A and z_B axes lie on the internuclear axis, pointing towards one another, the x and y axes are parallel and have the same direction.

2. Spherical coordinates centered on the nuclei A and B. In this case the NISTO's have the following expression:

$$\chi = N_{n\xi} r^{n-1} e^{-\xi r} Y_{lm}(\Omega)$$

3. Ellipsoidal coordinates with foci A and B. These coordinates are defined in terms of the spherical coordinates by

$$\xi = \frac{r_A + r_B}{AB} \qquad \eta = \frac{r_A - r_B}{AB} \qquad \varphi = \varphi_A = \varphi_B$$

the reciprocal relations are

$$r_A = \frac{AB}{2}(\xi + \eta) \qquad r_B = \frac{AB}{2}(\xi - \eta)$$

$$\cos\theta_A = \frac{1 + \xi\eta}{\xi + \eta} \qquad \cos\theta_B = \frac{1 - \xi\eta}{\xi - \eta}$$

In terms of ellipsoidal coordinates, the NISTO's are written:

$$\chi_a(\xi, \eta, \varphi) = N_{n_a\xi_a} \left(\frac{AB}{2}\right)^{n_a - 1} (\xi + \eta)^{n_a - 1}$$

$$e^{-(AB/2)(\xi+\eta)\xi_a} \mathscr{P}_{lm}\left(\frac{1 + \xi\eta}{\xi + \eta}\right) e^{im_a\varphi}$$

and $\chi_b(\xi, \eta, \varphi) = \chi_a(\xi, -\eta, \varphi)$.

4. One Electron Integrals

4.1. One-Electron Two-Center Integrals of the General Type $\langle \chi_a | M | \chi_b \rangle$

$M = 1$ for the overlap integrals,

$M = \frac{1}{r_A}$ or $\frac{1}{r_B}$ for the nuclear integrals, and

$M = -\frac{1}{2}\nabla^2$ for the kinetic integrals.

In the ellipsoidal coordinate system, the two-center charge distribution Ω_{AB} has following expression:

$$\Omega_{AB} = \chi_a\chi_b = N_{n_a\xi_a} N_{n_b\xi_b} (-1)^{m_a} \left(\frac{AB}{2}\right)^{n_a + n_b - 2} \left[\frac{(l_a - m_a)!}{(l_a + m_a)!} \frac{(l_b + m_b)!}{(l_b - m_b)!}\right]^{1/2}$$

$$(\xi+\eta)^{n_a-1}(\xi-\eta)^{n_b-1}\,e^{-\rho\xi}\,e^{-\tau\eta}\,\mathscr{P}_{l_a-m_a}\left(\frac{1+\xi\eta}{\xi+\eta}\right)+\mathscr{P}_{l_b m_b}\left(\frac{1-\xi\eta}{\xi-\eta}\right)e^{i(m_a+m_b)\varphi}$$

where $\rho = AB/2(\zeta_a + \zeta_b)$ and $\tau = AB/2(\zeta_a - \zeta_b)$.

The monoelectronic integrals are evaluated by double numerical integration over ξ and η of the expression

$$\int \Omega_{AB}\langle M\rangle\, dv = (-1)^{m_a}[(2l_a+1)(2l_b+1)]^{1/2}\left(\frac{AB}{2}\right)^{n_a+n_b+1}$$

$$\delta_{-m_a,m_b}\int_0^{\infty}\int_{-1}^{1}\omega\left(\frac{\xi}{\rho},\eta\right)^{n_a}\left(\frac{\xi}{\rho},-\eta\right)^{n_b}e^{-\xi}\,e^{-\tau\eta}\,P_{l_a,-m_a}\left(\frac{\xi}{\rho},\eta\right)$$

$$P_{l_b m_b}\left(\frac{\xi}{\rho},-\eta\right)\langle M\rangle\, d\eta\, d\xi$$

4.2. Nuclear Integrals $\left\langle \chi_a \left| \frac{1}{r_b} \right| \chi'_a \right\rangle$

In the spherical coordinates system, the one-center charge distribution Ω_{AA} has the following expression:

$$\Omega_{AA} = (-1)^{m_a} r_a^{n_a+n'_a-2}\,e^{-(\zeta_a+\zeta'_a)r_a}$$
$$\sum_{L=|l_a-l'_a|}^{l_a+l'_a}\left[\frac{(2l_a+1)(2l'_a+1)}{4(2L+1)}\right]^{1/2}\mathscr{C}_{L\;\;l_a l'_a}^{-m_a+m'_a\;\;-m_a m'_a}\,Y_{L,-m_a+m'_a}(\Omega_A)$$

Using the well-known Laplace expansion:

$$\frac{1}{r_b}=\sum_{\mu=0}^{\infty}\frac{4\pi}{2\mu+1}\frac{r_-^{\mu}}{r_+^{\mu+j}}\sum_{\sigma=-\mu}^{\mu}Y^*_{\mu\sigma}(\Omega_A)\,Y_{\mu\sigma}(\Omega_{AB})$$

where r_- and r_+ denote respectively the smaller and greater of r_a and AB, we find for the nuclear integral [9, 10]:

$$\left\langle \chi_a \left| \frac{1}{r_b} \right| \chi'_a \right\rangle = (-1)^{m_a}[(2l_a+1)(2l'_a+1)]^{1/2}$$
$$\sum_{\mu=|l_a-l'_a|}^{l_a+l'_a}\frac{1}{2\mu+1}\mathscr{C}_{\mu\;\;l_a l'_a}^{-m_a+m'_a\;\;-m_a m'_a}$$
$$\left[\frac{(\mu+m_a-m'_a)!}{(\mu-m_a+m'_a)!}\right]^{1/2}P_{\mu,-m_a+m'_a}(\cos\theta_{AB})$$
$$AB^{-(\mu+1)}(\zeta_a+\zeta'_a)^{-(n_a+n'_a+\mu+1)}\gamma(n_a+n'_a+\mu+1, AB(\zeta_a+\zeta'_a))$$
$$+AB^{-\mu}(\zeta_a+\zeta'_a)^{-(n_a+n'_a-\mu)}\Gamma(n_a+n'_a-\mu, AB(\zeta_a+\zeta'_a))$$

5. Hybrid and Coulomb Integrals

The potential U is derived from the one-center charge distribution (1):

$$\int \Omega_{AA} \frac{1}{r_{12}} dv_1 = (-1)^{m_a} \sum_{L=|l_a - l'_a|}^{l_a + l'_a} \frac{4\pi}{2L+1} \left[\frac{(2l_a+1)(2l'_a+1)}{4\pi(2L+1)} \right]^{1/2}$$

$$\mathscr{C}_{L\ l_a\ l'_a}^{M_a - m_a\ m'_a} Y_{L,M_a}(\Omega_{A_2})\, Z_a^{-(N_a+L+1)}\, r_{A_2}^{-(L+1)}\, \gamma(N_a + L + 1, Z_a r_{A_2})$$

$$+ Z_a^{-(N_a - L)}\, r_{A_2}^{L}\, \Gamma(N_a - L, Z_a r_{A_2})$$

where $Z_a = \zeta_a + \zeta'_a$

$M_a = -m_a + m'_a$

$M'_a = M_a - m''_a$

$N_a = n_a + n'_a$

This expression is obtained when $1/r_{12}$ is expanded around the center A with the Laplace-expansion by triple integration over the spherical harmonics [8].

The integration over the coordinates of the second electron is carried out numerically for the ξ and η ellipsoidal coordinates. The hybrid integral can then be written:

$$\left[\chi_a^* \chi'_a \left| \frac{1}{r_{12}} \right| \chi''^*_a \chi_b \right] = \tfrac{1}{2}(-1)^{m_a + m''_a} [(12l_a+1)(2l'_a+1)(2l''_a+1)$$

$$\times (2l_b+1)]^{1/2} \delta_{M'_a - m_b}$$

$$\sum_{L=|l_a - l'_a|}^{l_a + l'_a} \frac{1}{2L+1} \mathscr{C}_{L\ l_a\ l'_a}^{M_a - m_a\ m'_a} \sum_{L'=|L - l''_a|}^{L + l''_a} \mathscr{C}_{L'\ L\ l''_a}^{M'_a\ M_a - m''_a}$$

$$\left[\frac{(L' - M'_a)!}{(L' + M'_a)!} \frac{(l_b + M'_a)!}{(l_b - M'_a)!} \right]^{1/2} \left[Z_a^{-(N_a+L+1)} A_{L,L'} + Z_a^{-(N_a - L)} B_{L,L'} \right]$$

where the $A_{L,L'}$ and $B_{L,L'}$ auxiliary functions have the following form:

$$A_{L,L'} = \left(\frac{AB}{2} \right)^{n_b + n''_a - 2} \frac{e^{-\rho}}{\rho} \int_0^{\infty} \int_{-1}^{1} \omega\left(\frac{\xi}{\rho}, \eta \right)^{n''_a - L - 1} \omega\left(\frac{\xi}{\rho}, -\eta \right)^{n_b} e^{-\xi} e^{-\tau\eta}$$

$$\gamma\left(N_a + L + 1, \frac{Z_a AB}{2} \omega\left(\frac{\xi}{\rho}, \eta \right) \right) P_{L',M'_a}\left(\frac{\xi}{\rho}, \eta \right) P_{l_b, -M'_a}\left(\frac{\xi}{\rho}, -\eta \right) d\eta\, d\xi$$

and:

$$B_{L,L'} = \left(\frac{AB}{2} \right)^{n_b + n''_a + L + 1} \frac{e^{-\rho}}{\rho} \int_0^{\infty} \int_{-1}^{1} \omega\left(\frac{\xi}{\rho}, \eta \right)^{n''_a + L} \omega\left(\frac{\xi}{\rho}, -\eta \right)^{n_b} e^{-\xi}\, e^{-\tau\eta}$$

$$\Gamma\left(N_a - L, \frac{Z_a AB}{2} \omega\left(\frac{\xi}{\rho}, \eta \right) \right) P_{L',M'_a}\left(\frac{\xi}{\rho}, \eta \right) P_{l_b' - M'_a}\left(\frac{\xi}{\rho}, -\eta \right) d\eta\, d\xi$$

In the same way, we find the Coulomb integral:

$$\left[\chi_a\chi'_a\left|\frac{1}{r_{12}}\right|\chi_b\chi'_b\right] = \tfrac{1}{2}(-1)^{m_a+m_b}\left[(2l_a+1)(2l'_a+1)(2l_b+1)(2l'_b+1)\right]^{1/2}$$

$$\delta_{n'_a-n_b}\sum_{L_a=|l_a-l'_a|}^{l_a+l'_a}\frac{1}{2L_a+1}\mathscr{C}^{M_a\ -m_a\ m'_a}_{L_a\ \ l_a\ l'_a}\sum_{L_b=|l_b-l'_b|}^{l_b+l'_b}\mathscr{C}^{M_b\ -m_b\ m'_b}_{L_b\ \ l_b\ l'_b}$$

$$\left[\frac{(L_a-n_a)!\,(L_b+n_a)!}{(L_a+n_a)!\,(L_b-n_a)!}\right]^{1/2}Z_a^{-(N_a+L_a+L)}A'_{L_aL_b}+Z_a^{-(N_a-L_a)}B'_{L_aL_b}$$

and the auxiliary functions are:

$$A'_{L_aL_b}=\left(\frac{AB}{2}\right)^{N_b-L_a-1}\frac{e^{-Z_aAB/2}}{Z_bAB}\int_0^\infty\int_{-1}^{1}\omega\left(\frac{2\xi}{Z_bAB},\eta\right)^{-L_a}\omega\left(\frac{2\xi}{Z_bAB},-\eta\right)^{N_b-1}$$

$$e^{-\xi}\,e^{Z_bAB/2\eta}\gamma\left(N_a+L_a+1,\frac{Z_aAB}{2}\,\omega\left(\frac{2\xi}{Z_bAB},\eta\right)\right)$$

$$P_{L_aM_a}\left(\frac{2\xi}{Z_bAB},\eta\right)P_{L_b-M_a}\left(\frac{2\xi}{Z_bAB},-\eta\right)d\eta\,d\xi$$

and

$$B'_{L_aL_b}=\left(\frac{AB}{2}\right)^{n_b+L_a}\frac{e^{-Z_bAB/2}}{Z_bAB}\int_0^\infty\int_{-1}^{1}\omega\left(\frac{2\xi}{Z_bAB},\eta\right)^{L_a+1}\omega\left(\frac{2\xi}{Z_bAB},-\eta\right)^{N_b-1}e^{-\xi}\,e^{Z_bAB/2\eta}$$

$$\Gamma\left(N_a-L_a,\frac{Z_aAB}{2}\,\omega\left(\frac{2\xi}{Z_bAB},\eta\right)\right)P_{L_aM_a}\left(\frac{2\xi}{Z_bAB},\eta\right)P_{L_b-M_a}\left(\frac{2\xi}{Z_bAB},-\eta\right)d\eta\,d\xi$$

6. Evaluation of Exchange Integrals

Because of non-integer n, the Neumann expansion of $1/r_{12}$ in ellipsoidal coordinates would lead to rather complicated calculations. It is easier to translate the functions χ_b and χ'_b from center B to center A.

The following expansion is used to transfer a solid spherical harmonic [11, 12],

$$r_B^l Y_{lm}(\Omega_B)=\sum_{K=|m|}^{l}\left(\frac{2l+1}{2K+1}\right)^{1/2}p_K(lm)\,r_A^K AB^{l-K}Y_{Km}(\Omega_A)$$

where the constant p_K is defined by

$$p_K(lm)=\frac{(-1)^{K+m}}{(l-K)!}\left[\frac{(l+m)!}{(K+m)!}\,\frac{(l-m)!}{(K-m)!}\right]^{1/2}$$

The radial part of the orbital is also translated [13]:

$$r_B^\nu\,e^{-\zeta r_B}=\sqrt{2\pi}\sum_{\lambda=0}^{\infty}\frac{1}{r_AAB}B_\lambda^{\nu+1}(r_A,AB,\zeta)\,Y_{\lambda,0}(\Omega_A)$$

$$B_\lambda^n(r_A,AB,\zeta)=\int_{|AB-r_A|}^{AB+r_A}r_B^n\,e^{-\zeta r_B}\,\mathscr{P}_{\lambda,0}(\cos\theta_A)\,dr_B$$

Using the expansion of the normalized Legendre polynomial [5], we find the following auxiliary function:

$$B_\lambda^n(r_A, AB, \zeta) = [4r_A AB]^{-\lambda} \left(\frac{2\lambda+1}{2}\right)^{1/2}$$

$$\sum_{\nu=0}^{\lambda} \binom{\lambda}{\nu}^2 \int_{|AB-r_A|}^{AB+r_A} [(AB-r_A)^2 - r_B^2]^{\nu} [(AB+r_A)^2 - r_B^2]^{\lambda-\nu} e^{-\zeta r_B} r_B^n \, dr_B$$

which can be evaluated numerically. It is, however, faster to process algebraically.

Grouping the different terms, the final expression of the translated orbital is written:

$$\chi_b = \left(\frac{2l_b+1}{2}\right)^{1/2} \sum_{K=|m_b|}^{l_b} p_K(l_b m_b) \, r_A^{K-1} AB^{l_b-K-1} \sum_{\lambda=0}^{\infty} B^{n_b-l_b}(r_A, AB, \zeta_b)$$

$$\sum_{L_1=|K-\lambda|}^{K+\lambda} \left(\frac{2\lambda+1}{2K+1}\right)^{1/2} \mathscr{C}_{L_1 \; K \; \lambda}^{m_b \; m_b \; 0} Y_{L_1, m_b}(\Omega_A)$$

Therefore, the exchange integral is now:

$$\tfrac{1}{2}(-1)^{m_a+m'_b} AB^{l_b+l'_b-2} [(2l_a+1)(2l'_a+1)(2l_b+1)(2l'_b+1)]^{1/2}$$

$$\sum_{K_1=|m_b|}^{l_b} p_{K_1}(l_b - m_b) \, AB^{-K_1} \sum_{L_1=|l_a-l_b|}^{l_a+l_b} \mathscr{C}_{L_1}^{-m_a+m_b \; -m_a \; m_b} {}_{l_a \; l_b}^{\; l'_b} \sum_{K_2=|m'_b|}^{}$$

$$p_{K_2}(l'_b m'_b) \, AB^{-K_2} \sum_{L_2=|l'_a-l'_b|}^{l'_a+l'_b} \mathscr{C}_{L_2}^{m'_a-m'_b \; m'_a \; m'_b} {}_{l'_a \; l'_b} \sum_J \frac{1}{(2\nu+1)^2}$$

$$\sum_{\lambda=0}^{\infty} \sum_{\lambda'=0}^{\infty} \mathscr{C}_{\nu \qquad L_1 \; \lambda}^{-m_a+m_b \; -m_a+m_b \; 0} \mathscr{C}_{\nu \qquad L_2 \; \lambda}^{m'_a-m'_b \; m'_a-m'_b \; 0}$$

$$\beta_1^{-(n_a+n'_a+K_1+K_2+1)} \, 2^{-(n'_a+K_2+\nu+1)}$$

$$\int_0^{\infty} r_1^{n_a+K_1-\nu} e^{-r_1} B_\lambda^{n_b-l_b}\left(AB, \frac{r_1}{\beta_1}, \zeta_b\right) \int_{-1}^{1} (r_1 r_2 + r_1)^{n'_a+K_2+\nu}$$

$$e^{-\zeta'_a r_1 r_2/2\beta_1} B_{\lambda'}^{n'_b-l'_b}\left(AB, \frac{r_1 r_2 + r_1}{2\beta_1}, \zeta'_b\right) dr_2 \, dr_1$$

$$+ \zeta_a^{-1} \beta_2^{-(n_a+K_1+\nu+1)} \int_0^{\infty} r_l^{n_a+K_1+\nu} e^{-r_1} B_\lambda^{n_b-l_b}\left(AB, \frac{r_1}{\beta_2}, \zeta_b\right)$$

$$\int_0^{\infty} \left(\frac{r_1}{\beta_2} + \frac{r_2}{\zeta'_a}\right)^{n'_a+K_2-\nu-1} e^{-r_2} B_\lambda^{n'_b-l'_b}\left(AB, \frac{r_1}{\beta_2} + \frac{r_2}{\zeta'_a}, \zeta'_b\right) dr_2 \, dr_1$$

where $\beta_1 = \zeta_a + \zeta'_a/2$ and $\beta_2 = \zeta_a + \zeta'_a$.

7. SCF *ab initio* Calculation on LiH

As the non-integer n introduces a new variational parameter, it is interesting to study its effect on the calculation of a simple molecule like LiH with a minimal basis set, using the atomic parameters n which have been determined in our previous paper [1]:

Table 1. Orbital parameters

		η	ζ
Li	1s	0.99	2.67
	2s	2.01	0.622
	2p	1.590	0.622
H	1s	0.955	1.0

In an SCF *ab initio* calculation, the total energy of the molecule is −7.9666 a.u. if one uses an integer n and −7.9719 a.u. with a non-integer principal quantum number, i.e. a gain of about 0.1 eV.

Table 2. Molecular orbitals, energy levels and population analysis for an integer n

1s	2s	2p	h		
0.996572	0.016070	−0.005165	0.006043	−2.447140	
−0.130785	0.321922	0.236263	0.682761	−0.304386	
0.135029	−0.813999	0.588645	0.155701	0.133482	
−0.021862	0.862090	1.521706	−1.287360	0.351846	
				Mulliken Populations \ Energy Levels	
1.996	0.408	0.290	1.305		

Table 3. Molecular orbitals, energy levels and population analysis for a non-integer n

1s	2s	2p	h		
0.997165	0.021637	−0.007033	0.008022	−2.442340	
−0.124764	0.340077	0.256619	0.662912	−0.304135	
−0.124046	0.864879	−0.512707	−0.236372	0.002257	
0.000462	0.760320	1.129760	−1.238890	0.418706	
				Mulliken Populations \ Energy Levels	
1.997	0.428	0.317	1.257		

Going from Table 2 to Table 3, one can notice an important modification of the non-occupied energy levels and a flow of charge from the hydrogen to the lithium.

Table 4. Comparison with other works

Type of Calculation	Total Energy	References
Minimal NISTO Basis Set	−7.9719	This Work
One Center Wave Function	−7.9357	[14]
Minimal STO	−7.9699	[15]
14 GTO on Li 7 GTO on H	−7.9842	[16]
24 STO	−7.9873	[17]
Experimental	−8.075	[18]

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