Note

Computation of Molecular Integrals over Partially Generalized Hermite–Gaussian Functions

I. INTRODUCTION

Hermite–Gaussian functions (HG) as basis functions have been introduced by Živković and Maksić [1, 2]. Thereafter, these functions have been treated in a series of papers [3–10]. In particular, they widely used in X_α [11, 12] and in some ab initio calculations [13–15]. In addition, a method for the expansion charge distributions of the Cartesian Gaussian functions (CG) in terms of HG has been developed by McMurchie and Davidson [16] and Saunders [17]. We prefer, however, to build Hermite polynomials in the basis set functions from the very beginning. For that purpose we proposed and briefly discussed some generalizations of original HG function [18]. The idea behind this approach is that Hermite polynomials have some special properties which enable expression of many molecular integrals in a close form. Our preliminary calculations indicate that generalized HG functions deserve further tests and examination [19].

Hermite–Gaussian functions at a centre $\mathbf{A} = (A_x, A_y, A_z)$ are defined by [2]

$$
\begin{aligned}
f_{n_1, n_2, n_3}(a, \mathbf{r}_A) &= a^{-n/2}(\partial/\partial A_x)^{n_1} (\partial/\partial A_y)^{n_2} (\partial/\partial A_z)^{n_3} \exp(-a\mathbf{r}_A^2) \\
&= H_{n_1}(a^{1/2} x_A) H_{n_2}(a^{1/2} y_A) H_{n_3}(a^{1/2} z_A) \exp(-a\mathbf{r}_A^2),
\end{aligned}
\tag{1}
$$

where: $n = n_1 + n_2 + n_3$, $H_n(x)$ is the Hermite polynomial of the order n and $x_A = x - A_x$.

By distinguishing nonlinear parameters appearing in the polynomial and exponential parts, special generalized Hermite–Gaussian functions (SGHG) are obtained. They are defined in the following way

$$
\varphi_{n_1, n_2, n_3}(a, \mathbf{b}, \mathbf{r}_A) = H_{n_1}(b_1 x_A) H_{n_2}(b_2 y_A) H_{n_3}(b_3 z_A) \exp(-a\mathbf{r}_A^2).
\tag{2}
$$

By combining SGHG of the same exponential (a) and polynomial (b) parameters but of the different "quantum" numbers n_1, n_2, and n_3, composed Hermite–Gaussian functions (CHG) are obtained as follows:

$$
\begin{aligned}
\varphi^C_{n_1, n_2, n_3}(a, \mathbf{b}, \mathbf{r}_A) = \sum_{k_1=0}^{n_1} \sum_{k_2=0}^{n_2} \sum_{k_3=0}^{n_3} C_{k_1}(A_x) C_{k_2}(A_y) C_{k_3}(A_z) \\
\times \varphi_{k_1, k_2, k_3}(a, \mathbf{b}, \mathbf{r}_A).
\end{aligned}
\tag{3}
$$

474

Off-centre shift in the Hermite part of SGHG defines the third generalization of HG, i.e., Hermite off-centre Hermite–Gaussian functions (HOCHG):

$$\varphi^H_{n_1,n_2,n_3}(a, \mathbf{b}, \mathbf{p}_A) = H_{n_1}(b_1(x_A + p_1)) H_{n_2}(b_2(y_A + p_2)) H_{n_3}(b_3(z_A + p_3))$$
$$\times \exp(-a r_A). \tag{4}$$

In what follows three generalizations above (SGHG, CHG, HOCHG) of HG functions are called partially generalized Hermite–Gaussian functions (PGHG).

The further generalizations, like Gaussian off-centre shift Hermite and Guassian off-centre shift in SGHG an analogous generalizations for CGH, will not be considered here.

In the present paper, evaluation of the molecular integrals over PGHG functions is discussed, with particular emphasis on their performance and computational time saving.

II. EXPANSION OF TWO-CENTRE PRODUCT OF PGHG FUNCTIONS

The product of two PGHG functions located at generally two different centres **A** and **B** can be expanded in terms of HG functions located at the centre **P** in the following way:

$$H_n(bx_A) H_m(b'x_B) \exp(-ax_A^2 - a'x_B^2)$$
$$= \exp[-\delta(A_x - B_x)^2] \sum_{t=0}^{n+m} E_t(n, m, \gamma\, b, b', A_x, B_x, P_x) H_t(\gamma^{1/2} x_P) \exp(-\gamma x_P^2), \tag{5}$$

where: $P_x = (aA_x + a'B_x)/(a + a')$, $x_p = x - P_x$, $\gamma = a + a'$, and $\delta = aa'/(a + a')$.

Having in mind the orthogonality of Hermite polynomials, the expansion coefficients E_t are determined as:

$$E_t(n, m, \gamma, b, b', A_x, B_x, P_x)\pi^{1/2}2^t t! = \int_{-\infty}^{+\infty} H_n(bx_A) H_m(b'x_B) H_t(\gamma^{1/2}x_p)$$
$$\times \exp(-\gamma x_p^2) d(\gamma^{1/2}x_p), \tag{6}$$

and by further use of the formula:

$$H_n(x) = (\partial/\partial u)^n \exp(-u^2 + 2ux)|_{u=0}, \tag{7}$$

E_t's are given by:

$$E_t(n, m, \gamma, b, b', A_x, B_x, P_x) = \sum_{k=t}^{n+m} 2^{k-t} b'^k k!/t!$$

$$\times \left\{ \sum_{j=0}^{k-t} P_j \gamma^{-(j+t)/2} P_x^{k-j-t} \pi^{-1/2} \Gamma[(j+1)/2]/[j!(k-j-t)!] \right\}$$

$$\times \sum_{i=\max(0, k-m)}^{\min(n,k)} (b/b')^i \binom{n}{i}\binom{m}{k-i} H_{n-i}(-bA_x) H_{m-k+i}(-b'B_x), \qquad (8)$$

where: $P_j = (1(-1)^j)/2$ and Γ is gamma function.
In the special case of $P_x = 0$, Eq. (8) yields:

$$E_t(n, m, \gamma, b, b', A_x, B_x, 0) = P_{n+m+t} n! m! \sum_{i=0}^{[n/2]} \sum_{j=0}^{[m/2]} \sum_{k=0}^{[t/2]} (-1)^{i+j+t}$$

$$\times (2b)^{n-2i}(2b')^{m-2j} 2^{-2k} \gamma^{i+j-(n+m)/2}$$

$$\times \pi^{1/2} \Gamma[(n+m+t-2(i+j+k)+1)/2]/[i!j!k!$$

$$\times (n-2i)!(m-2j)!(t-2k)!], \qquad (9)$$

where $[t/2]$, the summation limit, denotes the largest integer less than or equal to $t/2$.

The recursion relation valid for the Hermite polynomials implies that the expansion coefficients E_t satisfy the following recursion relation in t and n:

$$bE_{t-1}(n-1, m, \gamma, b, b', A_x, B_x, P_x)$$

$$= E_t(n, m, \gamma, b, b', A_x, B_x, P_x) + (2bA_x - 2P_x)$$

$$\times E_t(n-1, m, b, b', A_x, B_x, P_x) - (n-1)E_t(n-2, m, \gamma, b, b', A_x, B_x, P_x).$$

$$(10)$$

An analogous recursion is valid in m as well.

The product of two SGHG functions located at generally two different centres **A** and **B** can be expanded in terms of HG functions located at the center **P**. The expansion is given by

$$\varphi_\mathbf{n}(a, \mathbf{b}, \mathbf{r}_A) \varphi_{\mathbf{n}'}(a', \mathbf{b}', \mathbf{r}_B) = \exp[-\delta(\mathbf{A} - \mathbf{B})^2]$$

$$\times \sum_{t_1=0}^{N_1} \sum_{t_2=0}^{N_2} \sum_{t_3=0}^{N_3} E_{t_1}(n_1, n_1', \gamma, b_1, b_1', A_x, B_x, P_x)$$

$$\times E_{t_2}(n_2, n_2', \gamma, b_2, b_2', A_y, B_y, P_y)$$

$$\times E_{t_3}(n_3, n_3', \gamma, b_3, b_3', A_z, B_z, P_z) f_t(\gamma, \mathbf{r}_P), \qquad (11)$$

where: $N_i = n_i + n_i'$, $i = 1, 2, 3$.

For the special case of $b_1 = b_2 = b_3 = a^{1/2}$ the above Equation reduces to the product of two HG functions.

An analogous procedure can be also applied for the CHG functions.

The expansion of the product of two CHG functions is formally equivalent to the above equation after the substitution of φ and E by φ^C and E^C, respectively,

$$E_t^C(n, m, \gamma, b, b', A_x, B_x, P_x) = \sum_{i=[0, t-m]}^{n} C_i(A_x) \sum_{j=[0, t-n]}^{m} C_j(B_x)$$
$$\times E_t(i, j, \gamma, b, b', A_x, B_x, P_x), \qquad (12)$$

where: $[p, r] = \max(p, r)$. The quantities $E_t(i, j, ...)$ are the same as in Eq. (8).

The use of Eq. (7) and Leibnitz's rule yields the following property of Hermite polynomials

$$H_n[b(x_A + p)] = \sum_{i=0}^{n} \binom{n}{i} (2bp)^{n-i} H_i(bx_A). \qquad (13)$$

By using it the product of two HOCHG functions is formally equivalent to Eq. (11) with the substitution of φ by φ^H and of the quantities E_t by E_t^H, where the latter

$$E_t^H(n, m, \gamma, b, b', p, p', A_x, B_x, P_x) = \sum_{i=[0, t-m]}^{n} \binom{n}{i} (2bp)^{n-i}$$
$$\times \sum_{j=[0, t-n]}^{m} \binom{m}{j} (2b'p')^{n'-j} E_t(i, j, \gamma, b, b', A_x, B_x, P_x). \qquad (14)$$

III. Overlap and Kinetic Energy Integrals over PGHG Functions

Following the procedure explained in Ref. [16] and the orthogonality of the Hermite polynomials the following formula for the overlap integral over PGHG functions is obtained

$$\langle \varphi_{\mathbf{n}'}^P(\mathbf{r}_A) \mid \varphi_{\mathbf{n}'}^P(\mathbf{r}_B) \rangle = (\pi/\gamma)^{3/2} E_0^P(n_1, n_1') E_0^P(n_2, n_2')$$
$$\times E_0^P(n_3, n_3') \exp[-\delta(\mathbf{A} - \mathbf{B})^2], \qquad (15)$$

where the upper index P refers to any of PGHG functions.

The kinetic energy integrals over PGHG can be expressed as the follwing linear combination of the overlap integrals over PGHG:

$$\langle \varphi_{\mathbf{n}}^P(\mathbf{r}_A) \mid -\Delta/2 \mid \varphi_{\mathbf{n}}^P(\mathbf{r}_B) \rangle = -1/2 \sum_{s=1}^{3} \sum_{i=0}^{2} q_s(i) \langle \varphi_{\mathbf{n}}^P(\mathbf{r}_A) \mid \varphi_{\mathbf{n}' + 2(1-i)\mathbf{u}_s}^P(\mathbf{r}_B) \rangle, (16)$$

where: $q_s(0) = a'^2/b_s'^2$, $q_s(1) = (2n_s' + 1)(a'^2/b_s'^2 - a')$, $q_s(2) = 4n_s'(n_s' - 1)(a'^2/b_s'^2 - 2a' + b_s'^2)$, $\mathbf{u}_1 = (1, 0, 0)$, $\mathbf{u}_2 = (0, 1, 0)$, and $\mathbf{u}_3 = (0, 0, 1)$.

Here, the upper index P refers to HG, SGHG, and HOCHG but not to CHG functions. The kinetic energy integrals over CHG can be, according to their definition, expressed as linear combinations of the overlap integrals over SGHG functions.

IV. Nuclear Attraction Integrals over PGHG Functions

The nuclear attraction integrals over PGHG functions are given by

$$
\begin{aligned}
\text{NAI} &\equiv \langle \varphi_{\mathbf{n}}^P(\mathbf{r}_A) \, | \, |\mathbf{r}_C|^{-1} | \, \varphi_{\mathbf{n}'}^P(\mathbf{r}_B) \rangle \\
&= 2\pi/\gamma \, \exp[-\delta(\mathbf{A}-\mathbf{B})^2] \sum_{k_1=0}^{N_1} \sum_{k_2=0}^{N_2} \sum_{k_3=0}^{N_3} (-1)^k E_{k_1}(n_1, n_1') \\
&\quad \times E_{k_2}^P(n_2, n_2') E_{k_3}^P(n_3, n_3') \, g(\mathbf{k}, \mathbf{K}),
\end{aligned}
\tag{17}
$$

where: $k = k_1 + k_2 + k_3$, $N_i = n_i + n_i'$, $i = 1, 2, 3$, and $\mathbf{K} = \gamma^{1/2}(\mathbf{C} - \mathbf{P})$.

The upper index P refers to any of PGHG functions. The functions g [2] (or the functions R_{NLM} in Refs. [16, 17]) are defined by

$$
g(\mathbf{k}, \mathbf{K}) = (\partial/\partial K_x)^{k_1} (\partial/\partial K_y)^{k_2} (\partial/\partial K_z)^{k_3} \int_0^1 \exp(-\mathbf{K}^2 s^2) \, ds,
\tag{18}
$$

and they can be expressed as an integral over an even polynomial and Gaussian function:

$$
g(\mathbf{k}, \mathbf{K}) = (-1)^k \int_0^1 \sum_{t=0}^{k} P_t(-1)^{t/2} 2^{k-t} C_t(\mathbf{k}, \mathbf{K}) s^{2k-t} \exp(-\mathbf{K}^2 s^2) \, ds,
\tag{19}
$$

with $P_t = (1 + (-1)^t)/2$. The coefficients C_t are given by

$$
\begin{aligned}
C_t(\mathbf{k}, \mathbf{K}) = k_1! \, k_2! \, k_3! & \sum_{i_1 = [0, \, t-k_2-k_3]}^{(k_1, t)} P_{i_1}/[(i_1/2)! \, (k_1-i_1)!] \\
& \times \sum_{i_2 = [0, \, t-i_1-k_3]}^{(k_2, t-i_1)} \frac{K_x^{k_1-i_1} K_y^{k_2-i_2} K_z^{k_3-t+i_1+i_2}}{(i_2/2)! \, [(t-i_1-i_2)/2]! \, (k_2-i_2)! \, (k_3-t+i_1+i_2)!},
\end{aligned}
\tag{20}
$$

where the symbol (p, r) appearing above the summation sign stands for $\min(p, r)$ and the symbol $[p, r]$ appearing below the summation sign stands for $\max(p, r)$.

The special cases of C_t appear when one, two, or all three components of $\mathbf{K}$ equal zero. Then, C_k's are given, respectively, by:

$$
\begin{aligned}
C_t(\mathbf{k}, K_x, K_y, 0) = P_{k_3}(-1)^{k_3/2} & k_1! \, k_2! \, k_3!/(k_3/2)! \\
& \times \sum_{i_1 = [0, \, t-k_2]}^{(k_1, t)} P_{i_1} K_x^{k_1-i_1} K_y^{k_2-t}/\{(i_1/2)! \, [(t-i_1)/2]! \\
& \times (k_1-i_1)! \, (k_2-t+i_1)!\};
\end{aligned}
\tag{21}
$$

$$C_t(\mathbf{k}, K_x, 0, 0) = P_{k_2} P_{k_3} (-1)^{(k_2 + k_3)/2} k_1! k_2! k_3! / [(k_2/2)!$$
$$\times (k_3/2)! (t/2)! (k_1 - t)!] K_x^{k_1 - t}; \tag{22}$$

$$C_t(\mathbf{k}, 0, 0, 0) = P_{k_1} P_{k_2} P_{k_3} (-1)^{(k_1 + k_2 + k_3)/2} k_1! k_2! k_3! /$$
$$[(k_1/2)! (k_2/2)! (k_3/2)!] \delta_{t,0}. \tag{23}$$

For the special case $\mathbf{K} = 0$ the function g is given by

$$g(\mathbf{k}, 0) = C_0(\mathbf{k}, 0, 0, 0)/(k_1 + k_2 + k_3 + 1). \tag{24}$$

Generally, the function g, expressed by Eq. (19) can be computed by only one numerical integration if the Rys quadrature [20] is used.

The same procedure can be used for the computation of the nuclear attraction integrals as well thus yielding:

$$\text{NAI} = 2\pi/\gamma \exp[-\delta(\mathbf{A} - \mathbf{B})^2] \int_0^1 Q_{2(n+n')}^P (s) \exp(-\mathbf{K}^2 s^2) \, ds. \tag{25}$$

Q is an even polynomial of the order $2(n_1 + n_2 + n_3 + n_1' + n_2' + n_3')$ in the integration variable s:

$$Q_{2(n+n')}^P(s) = \sum_{j=0}^{n+n'} s^{2j} S_j^P(\mathbf{n}, \mathbf{n}'). \tag{26}$$

The parametric coefficients S_j^P are the function of all input parameters,

$$S_j^P(\mathbf{n}, \mathbf{n}') = (-1)^j \sum_{k=j}^{(n+n', 2j)} (-1)^k 2^{2j-k} \sum_{k_1 = [0, k - N_2 - N_3]}^{(N_1, k)} E_{k_1}^P(n_1, n_1')$$
$$\times \sum_{k_2 = [0, k - k_1 - N_3]}^{(N_2, k - k_1)} E_{k_2}^P(n_2, n_2') E_{k - k_1 - k_2}^P(n_3, n_3') C_{2(k-j)}(\mathbf{k}, \mathbf{K}), \tag{27}$$

where $\mathbf{k} = (k_1, k_2, k - k_1 - k_2)$.

V. TWO–ELECTRON REPULSION INTEGRALS OVER PGHG FUNCTIONS

Two-electron repulsion integrals over PGHG functions are expressed as

$$\text{ERI} \equiv \langle \varphi_\mathbf{n}^P(\mathbf{r}_{A_1}); \varphi_{\mathbf{n}'}^P(\mathbf{r}_{B_1}) \, |r_{12}^{-1}| \, \varphi_{\mathbf{n}''}^P(\mathbf{r}_{C_2}); \varphi_{\mathbf{n}'''}^P(\mathbf{r}_{D_2}) \rangle$$
$$= G \sum_{t_1=0}^{N_1 + N_1'} \sum_{t_2=0}^{N_2 + N_2'} \sum_{t_3=0}^{N_3 + N_3'} \gamma_2^{t/2} g(\mathbf{t}, \mathbf{K}) A^P(t_1, n_1, n_1', n_1'', n_1''')$$
$$\times A^P(t_2, n_2, n_2', n_2'', n_2''') A^P(t_3, n_3, n_3', n_3'', n_3'''), \tag{28}$$

where

$$G = 2\pi^{5/2}(\gamma_1\gamma_2)^{-1}(\gamma_1 + \gamma_2)^{-1/2}\exp[-\delta_1(\mathbf{A}-\mathbf{B})^2 - \delta_2(\mathbf{C}-\mathbf{D})^2] \qquad (29)$$

and

$$A^P(r, n, n', n'', n''') = \sum_{i=[0,r-n''-n''']}^{(n+n',r)} (\gamma_1/\gamma_2)^{i/2} E_i^P(n, n') E_{r-i}^P(n'', n'''), \qquad (30)$$

where: $\gamma_1 = a + a'$, $\gamma_2 = a'' + a'''$, $\delta_1 = aa'/\gamma_1$, $\delta_2 = a''a'''/\gamma_2$, and $N_j = n_j + n_j'$, $N_j' = n_j'' + n_j'''$, $j = 1, 2, 3$.

The upper index P in (28) and (30) refers to any of PGHG functions. The function g in (28) has been already defined by Eq. (18). The meaning of other symbols in Eq. (28) is: $\mathbf{K} = \beta^{1/2}(\mathbf{P}-\mathbf{Q})$, $\beta = \gamma_1\gamma_2/(a + a' + a'' + a''')$, $\mathbf{P} = (a\mathbf{A} + a'\mathbf{B})/\gamma_1$, and $\mathbf{Q} = (a''\mathbf{C} + a'''\mathbf{D})/\gamma_2$.

In analogy with the nuclear attraction integrals two-electron repulsion integrals can be also computed using a numerical integration over an even polynomial (Rys quadrature) in the form

$$\text{ERI} = G \int_0^1 P_{2M}(s)\exp(-\mathbf{K}^2 s^2)\,ds, \qquad (31)$$

with

$$P_{2M}(s) = \sum_{j=0}^M S_j s^{2j} \qquad \text{and} \qquad M = n + n' + n'' + n'''. \qquad (32)$$

The coefficients S_j are given by

$$\begin{aligned}
S_j \equiv (-1)^j \sum_{k=j}^{(M,2j)} 2^{2j-k}\gamma_2^{k/2} & \sum_{t_1=[0,k-M_2-M_3]}^{(M_1,k)} \sum_{t_2=[0,k-t_1-M_3]}^{(M_2,k)} \\
& \times C_{2(k-j)}(t_1, t_2, k-t_1-t_2, \mathbf{K}) A^P(t_1, n_1, n_1', n_1'', n_1''') \\
& \times A^P(t_2, n_2, n_2', n_2'', n_2''') A^P(k-t_1-t_2, n_3, n_3', n_3'', n_3'''), \qquad (33)
\end{aligned}$$

where $M_i = N_i + N_i'$, $i = 1, 2, 3$, and $M = M_1 + M_2 + M_3$. The functions C and A have been defined in (20) and (30), respectively.

VI. COMPUTATIONAL CONSIDERATIONS

The overlap, kinetic energy, nuclear attraction, and two-electron repulsion integrals over SGHG and PGHG functions are expressed in terms of the coefficients E and E^P, respectively. Other one- and two-electron integrals can be expressed in this way as well [11].

Atomic basis sets may be represented by different PGHG functions. In building

up a computational program it is important to notice that the input ordinal number "I" of the basis function with the exponential parameters $a(I)$ determines all other parameters: $n_1(I)$, $n_2(I)$, $n_3(I)$, $b_1(I)$, ..., in which way the type of input basis function is defined.

Therefore it is useful to compute three matrices of the order three of E coefficients: $EX(I, J, K)$, $EY(I, J, K)$, and $EZ(I, J, K)$ before the ab initio calculation is performed. The loops over I, J follow the ordinal numbers of basis functions. The loops over K run from zero up to $n_1(I) + n_1(J)$, $n_2(I) + n_2(J)$ and $n_3(I) + n_3(J)$ for EX, EY, and EZ, respectively. It is also possible to store the most frequently used values of the function $\exp[-\delta(\mathbf{A} - \mathbf{B})]$ as a 2-dimensional matrix in order to save time.

Already determined E coefficients are needed for all types of molecular integrals. When the basis set is large enough then the calculation of all the above-mentioned quantities requires a small fraction of the total ab initio calculation time.

If the two-electron integral is calculated by use of Eq. (28) it requires the formation of matrices g for the function $g(t, \mathbf{K})$ (according to the method described in Refs. [16, 17]). When two-electron integrals are computed, first the coefficients A have to be calculated. If two-electron integrals are calculated by use of Eq. (31) calculation of the quantity A and the polynomial coefficients $S(J)$ is relquired. Afterward the numerical Rys quadrature is applied. Thus the two-electron integrals can be completely calculated by using numerical integration only once. This algorithm generally applies for all PGHG functions.

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