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Short Communication

An analytical expression for arbitrary derivatives of Gaussian functions exp(ax^2)

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In this study, an analytical expression for the arbitrary derivatives of Gaussian function e^{ax^2} is developed. Using this analytical expression developed within Rodrigues representation, an alternative expression is presented for the Hermite functions. With the help of the expression presented here the Hermite functions can easily be estimated.

Key words: Arbitrary derivatives, Gaussian functions, Hermite polynomial, Rodrigues representation.

INTRODUCTION

The notion of derivative which is an important topic of mathematics is used in physics, economics, statistics and engineering. It is possible to encounter the consecutive derivatives of the mathematical functions in science. The calculation of an arbitrary derivative of a mathematical function requires more mathematical operation and time. The more the value of derivative order, the more mathematical operation and time it requires. Thus, to have an analytical expression for an arbitrary derivative of a mathematical function will simplify a solution of problems and the coding this expression in computer programming language.

In electronic structure calculations of atoms, molecules and solids in linear combination of atomic orbital (LCAO) approximation, multicenter molecular integrals are encountered (Roothaan, 1951). The most common basis functions used in LCAO approximation are Salter type orbitals (STOs) and Gaussian type orbitals (GTOs). It is well-known that STOs describe electron density better than GTOs do. On the other hand, GTOs are preferred in physics research because of the easy calculation of their multicenter integrals. Therefore, there are several works devoted to calculation of Gaussian multicenter molecular integrals (as a function of) e^{ax^2} (Boys 1950; Fieck, 1980; Zivkovic, 1968; Brinkmann, 1991). The founder of the idea of using GTOs in multicenter molecular integrals, Boys (1950) suggested to calculate the calculation of multicenter molecular integrals over *s* functions and then differentiating these integral results with respect to the nuclear coordinates to obtain those over the higher angu-

$$\left\langle e^{-\alpha r_{A1}^2} \middle| \hat{O} \middle| e^{-\alpha r_{B1}^2} \right\rangle \text{ and}$$

$$\left\langle e^{-\alpha r_{A1}^2} e^{-\alpha r_{B1}^2} \middle| r_{12}^{-1} \middle| e^{-\alpha r_{C2}^2} e^{-\alpha r_{D}^2} \right\rangle,$$

lar momentum functions. The aim of this work is to obtain an expression for an arbitrary derivative of a Gaussian function e^{ax^2} for being useful in calculation of Gaussian molecular integrals and also in expressing mathematical functions that include Gaussian term in their mathematical structure. As an example, the obtained expression for arbitrary derivative of Gaussian function will be used in re-expressing new formula for the Hermite functions.

Expressions for some derivatives of function e^{ax^2} and generalization to any order.

Some derivatives of function e^{ax^2} according to x,

$\left(\frac{d^n}{dx^n} e^{ax^2} \right)$, are presented below:

1st derivative

$$\frac{d}{dx} e^{ax^2} = 2axe^{ax^2}, \tag{2.1}$$

2nd derivative

$$\frac{d^2}{dx^2}e^{ax^2} = 2ae^{ax^2}\left(1+2ax^2\right), \quad (2.2)$$

3rd derivative

$$\frac{d^3}{dx^3}e^{ax^2} = 4a^2xe^{ax^2}\left(2ax^2+3\right) \quad (2.3)$$

4th derivative

$$\frac{d^4}{dx^4}e^{ax^2} = 4a^2e^{ax^2}\left(3+12ax^2+4a^2x^4\right) \quad (2.4)$$

$$\frac{d^8}{dx^8}e^{ax^2} = 16a^4e^{ax^2}\left(105+840ax^2+840a^2x^4+224a^3x^6+16a^4x^8\right), \quad (2.5)$$

$$\frac{d^9}{dx^9}e^{ax^2} = 32a^5xe^{ax^2}\left(945+2520ax^2+1512a^2x^4+288a^3x^6+16a^4x^8\right). \quad (2.6)$$

We generalize the expression given above for derivatives from order 1 to 9 to order *n* by using Maple symbolic programming language (Heck, 2003) as in the following:

$$\frac{d^n}{dx^n}e^{ax^2} = e^{ax^2}\sum_{i=0}^{n}{}^{(2)}C_{it}^n(\alpha)x^m . \quad (2.7)$$

Here the symbol $\sum^{(2)}$ indicates that the summation is to be performed in steps of two and the summation coefficient $C_{it}^n(\alpha)$ is presented as

$$C_{it}^n(\alpha) = \frac{(2\alpha)^t}{1+i\varepsilon_n^+}F_i(n)\left[(n-i)-\varepsilon_n^+\right]!! \quad (2.8)$$

With

$$m = i+\varepsilon_n^- , \quad (2.9)$$

$$\varepsilon_n^{\pm} = \frac{1}{2}\left[1\pm(-1)^n\right], \quad (2.10)$$

$$t = \frac{(n+i)}{2}+\varepsilon_n^- , \quad (2.11)$$

The symbol $F_i(n)$ in (2.8) is known as the binomial coefficient defined by

$$F_i(n) = \frac{n!}{i!(n-i)!} \quad (2.12)$$

As is seen from (2.7)-(2.12), the obtained expression for arbitrary derivative of Gaussian functions is very simple and can be coded easily to compute in any programming language.

As an application of the expression of arbitrary derivative for Gaussian functions we presented here with (2.7), we want to obtain a simple expression for the Hermite functions. Rodrigues representation of the Hermite functions (Arfken, 2001) which is a special function of mathematics and used in many physical problems, is as follows:

$$H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}\left(e^{-x^2}\right) \quad (2.13)$$

Substituting (2.7) into (2.13), an alternative expression can be presented for the Hermite function as follows:

$$H_n(x) = \sum_{i=0}^{n}{}^{(2)}(-1)^{t+n}C_{it}^n(1)x^m . \quad (2.14)$$

RESULTS AND DISCUSSIONS

We presented a simple expression for arbitrary derivative of Gaussian function $e^{\alpha x^2}$ in this paper. The obtained expression includes binomial coefficients and double factorials, and therefore can be programmed easily in computer. As an example of this expression we developed an alternative expression for the Hermite functions using Rodrigues representation. The Hermite functions can be easily obtained by using (2.7). Some of the Hermite functions are presented in Table 1. The current study is likely to be useful in calculation of multicenter molecular integrals over GTOs and electronic structural calculations of

Table 1. Some Hermite Polynomials Obtained using (2.14).

n	$H_n(x)$	n	$H_n(x)$
0	$H_0(x)=1$	5	$H_5(x)= 32x^5 -160x^3 +120x$
1	$H_1(x)= 2x$	6	$H_6(x)=64x^6 -480x^4 +720x^2 -120$
2	$H_2(x)= 4x^2 -2$	7	$H_7(x)=128x^7 -1344x^5 +3360x^3 -1680x$
3	$H_3(x)= 8x^3 -12x$	8	$H_8(x)= 256x^8 -3584x^6 +13448x^4 -13440x^2 +1680$
4	$H_4(x)=16x^4 -48x^2 +12$	9	$H_9(x)=512x^9 -9216x^7 +48364x^5 -80640x^3 +30240x$

atoms, molecules and solids with GTOs as basis functions.

Work is in progress for the calculation of multicenter molecular integrals over GTOs using the procedure presented in this paper.

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