Evaluation of multicenter electronic attraction, electric field and electric field gradient integrals with screened and nonscreened Coulomb potentials over integer and noninteger *n* slater orbitals

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By the use of complete orthonormal sets of Ψ^α-exponential-type orbitals, where $(\alpha = 1, 0, -1, -2, \dots)$ the multicenter electronic attraction (EA), electric field (EF) and electric field gradient (EFG) integrals of nonscreened and Yukawa-like screened Coulomb potentials are expressed through the two-center overlap integrals with the same screening constants and the auxiliary functions $\bar{Q}^q_{-NN}$ introduced in our previous paper (I.I. Guseinov, J. Phys. B, 3 (1970) 1399). The recurrence relations for auxiliary functions are useful for the calculation of multicenter EA, EF and EFG integrals for arbitrary integer and noninteger values of principal quantum numbers, screening constants, and location of slater-type orbitals. The convergence of the series is tested by calculating concrete cases.

KEY WORDS: screened Coulomb potentials, multicenter electric field integrals, multicenter electric field gradient integrals, noninteger principal quantum numbers

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1. Introduction

It is well known that the nuclear dynamic shielding constants, the forces exerted by the electrons on the nuclei and electron–nuclei quadrupole interactions for molecules obtained from the electronic attraction potentials and their derivatives with respect to Cartesian coordinates of nuclei are very sensitive to the minor errors in the wave functions [1]. Therefore, for the calculations of these

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properties it is desirable to use slater-type orbitals (STOs) as basis sets which describe the physical situation more accurately than do Gaussian-type orbitals (GTOs). However, the difficulties in calculating multicenter integrals have restricted the use of STOs in structure calculations of molecules.

The earliest approaches for the evaluation of multicenter integrals consisted of using the relatively complicated addition theorems of STOs to separate the integration variables from those related to the geometry of the molecule [2–18]. The great progress made in both applied mathematics and computer science has led a number of researchers to focus their efforts on the elaboration of new approaches directed to computing multicenter integrals over STOs. Unfortunately, they also were not entirely successful. To our knowledge, many authors (see [19–23] and references therein) have addressed this problem and although many improvements have been made in past few years by the use of computers, an efficient general program for the calculation of multicenter integrals over STOs is not yet available so far. We have had considerable success in using the addition theorems in the evaluation of multicenter molecular integrals. In [24], by the use of complete orthonormal sets of Ψ^α-exponential-type orbitals (ETOs) introduced in [25] all the multicenter multielectron integrals with integer and noninteger n STOs were expressed in terms of overlap integrals between the basis functions and the integer n STOs being translated. For the calculation of overlap integrals of integer and noninteger n STOs efficient computer programs are available in our group [26–28].

Therefore, by using the computer programs for the overlap integrals one can calculate the arbitrary multicenter integrals with integer and noninteger n STOs appearing in the determination of various properties for molecules when the Hartree–Fock–Roothaan approximation is employed.

In the Hartree–Fock–Roothaan approximation for molecules, the matrix elements of electronic attraction (EA), electric field (EF) and electric field gradient (EFG) operators between the determinantal wave functions are expressed through the multicenter integrals with the same operators. The multicenter integrals over STO are examined in this work have the following form:

Multicenter EA integrals

$$U_{p^*p'^*}(\eta, \zeta, \zeta'; \vec{R}_{cb}, \vec{R}_{ab}) = \int O(\eta, r_{a1}) \chi_{p^*}(\zeta, \vec{r}_{b1}) \chi_{p'^*}^*(\zeta', \vec{r}_{c1}) \, dV_1. \qquad (1)$$

Multicenter EF integrals

$$U_{p^*p'^*}^i(\eta, \zeta, \zeta'; \vec{R}_{cb}, \vec{R}_{ab}) = \int O^i(\eta, \vec{r}_{a1}) \chi_{p^*}(\zeta, \vec{r}_{b1}) \chi_{p'^*}^*(\zeta', \vec{r}_{c1}) \, dV_1. \qquad (2)$$

Multicenter EFG integrals

$$U_{p^*p'^*}^{ij}(\eta, \zeta, \zeta'; \vec{R}_{cb}, \vec{R}_{ab}) = \int O^{ij}(\eta, \vec{r}_{a1}) \chi_{p^*}(\zeta, \vec{r}_{b1}) \chi_{p'^*}^*(\zeta', \vec{r}_{c1}) \, dV_1, \qquad (3)$$

where $\eta \geqslant 0$, $i, j = 1, -1, 0$; $p^* \equiv n^*lm$, $p'^* \equiv n^{*\prime}l'm'$, $\vec{R}_{cb} = \vec{r}_{c1} - \vec{r}_{b1}$, $\vec{R}_{ab} = \vec{r}_{a1} - \vec{r}_{b1}$ and O, O^i and O^{ij} are EA, EF and EFG operators determined by

$$O(\eta, r_{a1}) = \frac{\mathrm{e}^{-\eta r_{a1}}}{r_{a1}} \tag{4}$$

$$O^i(\eta, \vec{r}_{a1}) = \frac{\partial}{\partial X^i} O(\eta, r_{a1}) = \frac{x_{a1}^i}{r_{a1}^3}(1 + \eta r_{a1})\mathrm{e}^{-\eta r_{a1}} \tag{5}$$

$$O^{ij}(\eta, \vec{r}_{a1}) = \frac{\partial^2}{\partial X^i \partial X^j} O(\eta, r_{a1}) = \frac{3x_{a1}^i x_{a1}^j - \delta_{ij} r_{a1}^2}{r_{a1}^5}\left(1 + \eta r_{a1} + \frac{\eta^2}{3}r_{a1}^2\right)\mathrm{e}^{-\eta r_{a1}}$$
$$+ \frac{\eta^2 \mathrm{e}^{-\eta r_{a1}}}{3r_{a1}}\delta_{ij} - \frac{4\pi}{3}\delta_{ij}\delta(\vec{r}_{a1}). \tag{6}$$

Here $x^1 = x$, $x^{-1} = y$, $x^0 = z$ and $X^1 = X$, $X^{-1} = Y$, $X^0 = Z$ are the Cartesian coordinates of the electron and nucleus a, respectively; $\delta(\vec{r})$ is the Dirac delta function; $\chi_{p^*}(\zeta, \vec{r}_{b1})$ and $\chi_{p'^*}(\zeta', \vec{r}_{c1})$ are normalized real or complex noninteger n STOs centered on nuclei b and c, respectively:

$$\chi_{n^*lm}(\zeta, \vec{r}) = (2\zeta)^{n^*+1/2}[\Gamma(2n^* + 1)]^{-1/2} r^{n^*-1}\mathrm{e}^{-\zeta r} S_{lm}(\theta, \varphi). \tag{7}$$

Here $\Gamma(x)$ denotes the gamma function [29]. The normalized integer n STOs can be obtained from equation (7) for $n^* = n$, where n is an integer:

$$\chi_{nlm}(\zeta, \vec{r}) = (2\zeta)^{n+1/2}[(2n)!]^{-1/2}r^{n-1}\mathrm{e}^{-\zeta r} S_{lm}(\theta, \varphi). \tag{8}$$

The aim of this report is to obtain the series expansion formulas for the multi-center EA, EF and EFG integrals, equations (1)–(3), through the overlap integrals with the arbitrary integer and noninteger values of principal quantum numbers of STOs and the auxiliary functions.

2. Expressions for multicenter EA, EF and EFG integrals in terms of two-center basic integrals and auxiliary functions

In order to evaluate the multicenter EA, EF and EFG integrals, equations (1)–(3), we first use the following series expansion formulas for the electron charge densities with the noninteger n STOs in terms of integer n STOs at the displaced center:

$$\chi_{p^*}(\zeta, \vec{r}_b)\chi_{p'^*}^*(\zeta', \vec{r}_c) = \frac{1}{\sqrt{4p}} \lim_{N \to \infty} \sum_{\mu=1}^{N}\sum_{\nu=0}^{\mu-1}\sum_{\sigma=-\nu}^{\nu} W_{p^*p'^*q}^{\alpha N}(\zeta, \zeta', z; \vec{R}_{cb}, 0)\chi_q(z, \vec{r}_b),$$
$$\tag{9}$$

where $\alpha = 1, 0, -1, -2, \ldots, p^* \equiv n^*lm, p'^* \equiv n'^*l'm', q \equiv \mu\nu\sigma$ and $z = \zeta + \zeta'$; the quantities $W^{\alpha N}_{p^*p'^*q}(\zeta, \zeta', z; \vec{R}_{cb}, 0)$ are the two-center charge density expansion coefficients which can be expressed through the two-center overlap integrals with the same screening parameters (see equations (6) and (14) of [24]). The expressions of overlap integrals with integer and noninteger principal quantum numbers of STOs are given in [30,31].

Using equation (9) in equations (1)–(3), we obtain the series expansion formulas for the multicenter EA, EF and EFG integrals in terms of two-center basic integrals defined by

$$J_q(\eta, z; \vec{R}) = \frac{1}{\sqrt{4\pi}} \int O^*(\eta, r_{a1}) \chi_q(z, \vec{r}_{b1}) \, dV_1, \tag{10}$$

$$J_q^i(\eta, z; \vec{R}) = \frac{\partial}{\partial X^i} J_q(\eta, z; \vec{R}) = \frac{1}{\sqrt{4\pi}} \int O^i(\eta, \vec{r}_{a1}) \chi_q(z, \vec{r}_{b1}) \, dV_1 \tag{11}$$

$$J_q^{ij}(\eta, z; \vec{R}) = \frac{\partial}{\partial X^i} J_q^j(\eta, z; \vec{R}) = \frac{1}{\sqrt{4\pi}} \int O^{ij}(\eta, \vec{r}_{a1}) \chi_q(z, \vec{r}_{b1}) \, dV_1, \tag{12}$$

where $\vec{R} = \vec{R}_{ab}$.

Taking into account equation (15) of [32] in equation (10), it is easy to establish for the two-center basic EA integrals the following relation:

$$J_{\mu\nu\sigma}(\eta, z; \vec{R}) = (-1)^\nu \frac{N_{0\mu}(p, t)}{\sqrt{2\eta}} \sum_{\beta=0}^{\nu} \sum_{q=0}^{\beta} \bar{g}_{0\beta}^q(00, \nu 0) \bar{Q}_{0,\mu-\beta}^q(p, t) \bar{S}_{\nu\sigma}(\theta, \varphi), \tag{13}$$

where $p = R(\eta + z)/2, t = (\eta - z)/(\eta + z)$,

$$N_{0\mu}(p, t) = \frac{[p(1+t)]^{1/2}[p(1-t)]^{\mu+1/2}}{\sqrt{(2\mu)!}},$$

$$\bar{S}_{\nu\sigma}(\theta, \varphi) = \left(\frac{4\pi}{2\nu+1}\right)^{1/2} S_{\nu\sigma}(\theta, \varphi),$$

$$Q_{-NN'}^q(p, t) = \int_1^\infty \int_{-1}^1 \frac{(1+\mu\nu)^q(\mu-\nu)^{N'}}{(\mu+\nu)^N} e^{-p\mu-pt\nu} \, d\mu \, d\nu, \tag{14}$$

$$\bar{g}_{\alpha\beta}^q(l\lambda, l'\lambda) = g_{\alpha\beta}^0(l\lambda, l'\lambda) 2^{\alpha+\beta-q} F_{q-\alpha-\lambda}(0, \beta-\lambda). \tag{15}$$

See [33] for the exact definition of the coefficients $g_{\alpha\beta}^q(l\lambda, l'\lambda)$.

Using equation (5) in equation (11) for the two-center basic EF integrals we obtain

$$J_{\mu\nu\sigma}(\eta, z; \vec{R}) = \sum_{u=-1}^{0} \eta^{u+1} F_{u1i,\mu\nu\sigma}(\eta, z; \vec{R}). \tag{16}$$

Here $F_{uvs,\mu v\sigma}(\eta, z; \vec{R})$ are the two-center overlap integrals between potential functions [34]

$$f_{uvs}(\eta, \vec{r}) = r^{u-1}e^{-\eta r}\bar{S}_{vs}(\theta, \varphi) \tag{17}$$

and STOs defined by

$$F_{uvs,\mu v\sigma}(\eta, z; \vec{R}) = \frac{1}{\sqrt{4\pi}} \int f_{uvs}^*(\eta, \vec{r}_{a1})\chi_{\mu v\sigma}(z, \vec{r}_{b1})\,dv_1, \tag{18}$$

where $v = 0, 1, 2, \ldots, -v \leqslant s \leqslant v$ and $u \geqslant -v$.

Now we can move on to the evaluation of two-center overlap integrals, equation (18). For this purpose we take into account the expansion formulas for rotational transformation of overlap integrals with the arbitrary atomic orbitals [35]. Then we obtain with respect to molecular coordinate system (unlined coordinate systems) the following relation:

$$F_{uvs,\mu v\sigma}(\eta, z; \vec{R}) = \sum_{\lambda=0}^{\min(v,v)} T_{vs,v\sigma}^{\lambda}(\theta, \varphi)F_{uv\lambda,\mu v\lambda}(\eta, z; R), \tag{19}$$

where the functions $F_{uv\lambda,\mu v\lambda}(\eta, z; R)$ are determined in the lined-up coordinate systems. See [35] for the exact definition of rotation coefficients $T_{vs,v\sigma}^{\lambda}(\theta, \varphi)$.

For the evaluation of two-center basic EFG integrals, equation (12), we should obtain the derivatives of EF integrals with respect to Cartesian coordinates of nucleus a. For this purpose we utilize the method set out in [36]. Then, we can express all of the two-center basic EA, EF and EFG integrals in terms of common potential function, namely:

$$J_{\mu v\sigma}(\eta, z; \vec{R}) = F_{000,\mu v0,v\sigma}^{0,00}(\eta, z; \vec{R}), \tag{20}$$

$$J_{\mu v\sigma}^{i}(\eta, z; \vec{R}) = \sum_{u=-1}^{0} \eta^{u+1} \sum_{\lambda=0}^{\min(1,v)} \frac{2}{(1+\delta_{\lambda0})[(1+\delta_{i0})(1+\delta_{\sigma0})]^{1/2}}$$

$$\times \sum_{k=-1}^{1}{}^{(2)} \sum_{L=|1-v|}^{1+v} (\varepsilon_{i0})^{\delta_{k,\varepsilon_{i\sigma}}} C_{k\gamma,\gamma',k\gamma+\gamma'}^{1vL} C_{\lambda,-\lambda,0}^{1vL} \left(\frac{1+\delta_{M_k0}}{2}\right)^{1/2}$$

$$\times F_{u1\lambda,\mu v\lambda,LM_k}^{0,00}(\eta, z; \vec{R}), \tag{21}$$

$$J_{\mu v\sigma}^{ij}(\eta, z; \vec{R}) = \sum_{u=-1}^{0} \eta^{u+1} \sum_{\lambda=0}^{\min(1,v)} \sum_{k=-1}^{1}{}^{(2)} \sum_{L=|1-v|}^{1+v} (\varepsilon_{j0})^{\delta_{k,\varepsilon_{j\sigma}}}$$

$$\times \frac{(\varepsilon_{j0})^{\delta_{k,\varepsilon_{j\sigma}}}[2(1+\delta_{M_k0})]^{1/2}}{(1+\delta_{\lambda0})[(1+\delta_{j0})(1+\delta_{\sigma0})]^{1/2}} C_{k\gamma,\gamma',k\gamma+\gamma'}^{1vL}$$

$$\times C^{1\upsilon L}_{\lambda,-\lambda,0} \left\{ \sum_{m=-(L-1)}^{L-1} a^i_{LM_k,m} F^{1,00}_{u1\lambda,\mu\nu\lambda,L-1m}(\eta, z; \vec{R}) \right.$$

$$+ \left(\frac{X^i}{R}\right)[(u+\mu-L+1)F^{1,00}_{u1\lambda,\mu\nu\lambda,LM_k}(\eta, z; \vec{R})$$

$$-\frac{1}{2}p(1+t)\mathrm{F}^{1,10}_{u1\lambda,\mu\nu\lambda,LM_k}(\eta, z; \vec{R})$$

$$\left. -\frac{1}{2}p(1-t)F^{1,01}_{u1\lambda,\mu\nu\lambda,LM_k}(\eta, z; \vec{R})] \right\} - \frac{\sqrt{4\pi}}{3}\chi_{\mu\nu\sigma}(\zeta, -\vec{R})\delta_{ij}, \qquad (22)$$

where $\gamma = |j|$, $\gamma' = |\sigma|$ and $M_k = \varepsilon_{j\sigma}|k\gamma + \gamma'|$. The quantities $F^{a,kk'}_{u\upsilon\lambda,\mu\nu\lambda,LM}(\eta, z; \vec{R})$ occurring in equations (20)–(22) are the noncentral potential functions the central parts of

$$F^{a,kk'}_{u\upsilon\lambda,\mu\nu\lambda,LM}(\eta, z; \vec{R}) = F^{a,kk'}_{u\upsilon\lambda,mu\nu\lambda}(\eta, z; R)\bar{S}_{LM}(\theta, \varphi) \qquad (23)$$

are determined in terms of auxiliary functions $\bar{Q}^q_{-NN'}$ by the relation

$$F^{a,kk'}_{u\upsilon\lambda,\mu\nu\lambda}(\eta, z; R) = F^{a,kk'}_{u\upsilon\lambda,\mu\nu\lambda,00}(\eta, z; R) = (-1)^\nu \frac{N_{u\mu}(p,t)}{3^{1/\upsilon}(2\eta)^{u+1/2}R^a}$$

$$\times \sum_{\alpha=-\lambda}^{\upsilon} \sum_{\beta=\lambda}^{\nu} \sum_{q=\alpha+\lambda}^{\alpha+\beta} \bar{g}^q_{\alpha\beta}(\upsilon\lambda, \nu\lambda)\bar{Q}^q_{u-\lambda+k,\mu-\beta+k'}(p,t), \qquad (24)$$

where

$$N_{u\mu}(p,t) = \frac{[p(1+t)]^{u+1/2}[p(1-t)]^{\mu+1/2}}{\sqrt{(2\mu)!}}. \qquad (25)$$

For $\gamma = \gamma'$ and $\varepsilon_{j\sigma} = -1$ terms with a negative value of index $k(k = -1)$ contained in equation (22) should be equated to zero. We notice that the symbol $\varepsilon_{j\sigma}$ in equation (22) may have the values ± 1 and is determined by the product of the signs j and σ (the sign of zero is regarding as positive). The quantities C in equations (21) and (22) are the Clebsch–Cordan coefficients in the case of our phases ($Y^*_{lm} = Y_{l-m}$, see [33]):

$$C^{ll'L}_{mm'M} = (-1)^{1/2(m+|m|+m'+|m'|+M+|M|)}(ll'mm'/ll'LM), \qquad (26)$$

where $(ll'mm'/ll'LM)$ is a Clebsch–Cordan coefficients in Condon–Shortley phases.

For the computation of auxiliary functions $\bar{Q}^q_{-NN'}(p,t)$ occurring in equation (24), we can use the following recurrence relations [23]:

For lowering the indices N

$$2(N-1)\bar{Q}^q_{-NN'} = -p(1+t)\bar{Q}^q_{-N+1N'} + q\bar{Q}^{q-1}_{-N+2N'} + J^{+1q}_{q-N+1N'}. \tag{27}$$

For lowering the indices N'

$$2N'\bar{Q}^q_{-N+1N'-1} = p(1-t)\bar{Q}^q_{-N+1N'} + q\bar{Q}^{q-1}_{-N+1N'+1} + J^{-1q}_{q-N+1N'}. \tag{28}$$

See [28] for the exact definition of $J^{\pm1q}_{q-N+1N'}$. By the use of recurrence relation [27], the calculation of auxiliary function $\bar{Q}^q_{-NN'}$ can be reduced to the calculation of the function $\bar{Q}^q_{-1N'}$ determined by

$$\bar{Q}^q_{-1N'} = \sum_{q'=0}^{q} F_{q'}(q) Q^q_{-1N'}. \tag{29}$$

Here $Q^q_{-1N'}$ determined by

$$Q^q_{-1N'}(p, t) = \sum_{\sigma=0}^{N'+q} \eta^q_{N'\sigma}[A_{N'+2q-\sigma}(p-pt)h_\sigma(2pt) - (-1)^\sigma f_\sigma(2p)$$

$$-(-1)^{N'} A_{N'+2q-\sigma}(-p+pt)A_{\sigma-1}(2p)], \tag{30}$$

where

$$A_k(p) = \int_1^\infty \mu^k e^{-p\mu}\,d\mu, \tag{31}$$

$$B_k(pt) = \int_{-1}^1 v^k e^{-ptv}\,dv, \tag{32}$$

$$\eta^q_{N'\sigma} = (-1)^q \sum_{k=0}^{q} 2^k F_k(q) F_{\sigma-k}(N'), \tag{33}$$

$$h_\sigma(x) = \begin{cases} -A_{\sigma-1}(x) + f_\sigma(x) & \text{for } x \neq 0, \ \sigma \neq 0, \\ Ei(-x) - \ln(x) & \text{for } x \neq 0, \ \sigma = 0, \\ 1/\sigma & \text{for } x = 0, \ \sigma \neq 0, \\ C & \text{for } x = 0, \ \sigma = 0, \end{cases} \tag{34}$$

$$f_\sigma(x) = \begin{cases} (\sigma-1)/x^\sigma & \text{for } x \neq 0, \ \sigma \neq 0, \\ -\ln|x| & \text{for } x \neq 0, \ \sigma = 0. \end{cases} \tag{35}$$

Here C is the Euler constants and $Ei(-x)$ is an exponential integral defined by [29],

$$Ei(-x) = -\int_x^\infty \frac{e^{-t}}{t}\,dt. \tag{36}$$

As can be seen from the formulas obtained in this work, all the multicenter EA, EF and EFG integrals can be calculated using equations (23) and (24) for potential functions. For this purpose we need only the Cartesian coordinates of the nuclei of a molecule need only the quantum numbers, screening constants and location of STOs.

3.   Numerical results and discussion

On the basis of analytical relations [1–3] for multicenter EA, EF and EFG and [20–23] for the basic integrals we constructed a program. These programs can be used in the calculation of multicenter EA, EF and EFG integrals over integer and noninteger n STOs. The results of calculations in atomic units for the multicenter EF and EFG integrals in molecular coordinate system on a pentium III 800 MHz (using Turbo Pascal language) are represented in Table 1.

The computer time required for the calculation of calculation of multicenter nuclear-attraction and electron repulsion integrals are not given in the tables due to the fact that the comparison cannot be made with the different computers used in the literature. It is seen from the algorithm presented for multicenter integrals that our CPU times are satisfactory. For instance, for two-center nuclear-attraction integrals with quantum sets $n^* = 2$, $l = 1$, $m = 1$, $\zeta = 7.4$, $n'^* = 1$, $l' = 0$, $m' = 0$, $\zeta' = 4.2$ and $\eta = 2.1$ CPU time takes about 17.5 ms.

The comparative values obtained from equations (2) and (3) with the expansion of different Ψ^α-ETOs, are shown in these tables. We see from the tables that the accuracy of computer results for different expansion formulas obtained from Ψ^0-ETOs and Ψ^1-ETOs is satisfactory.

Table 1

The values of three-center EF and EFG integrals in molecular coordinate system for $X^1 = -0.7$, $X^{-1} = -0.2$, $X^0 = 0.43$ (in a.u.).

| | | | | | | | | | | | Equations (2) and (3) for $N = 13$ | |
n^*	l	m	ζ	n'^*	l'	m'	ζ'	η	i	j	$\alpha = 0$	$\alpha = 1$
2	1	1	7.4	1	0	0	4.2	2.1	−1		4.91349953E−03	4.91351993E−03
2	1	1	3.4	2	1	0	5.4	1.7	0		−2.91711988E−02	−2.91714916E−02
2	1	1	6.3	2	1	1	3.5	0.1	1		−7.20342412E−02	−7.20345691E−02
2	1	−1	8.5	2	1	1	6.3	0.5	1		4.69234519E−03	4.69309431E−03
2.5	1	0	3.7	1.8	0	0	1.5	0.8	−1		8.24407704E−03	8.24573279E−03
2	1	0	4.7	1	0	0	2.3	1.5	−1	0	6.06406925E−02	6.06428667E−02
1.5	0	0	5.7	1.8	0	0	3.7	1.5	−1	0	−1.16181489E−02	−1.16173765E−02

Results obtained with the following geometry (Cartesian coordinates): $b(0.7, 0.2, -0.43)$, $c(-0.4, 1.2, -0.18)$, $a(0, 0, 0)$.

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