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RESEARCH ARTICLE

Three-Center One-Electron Molecular Integrals over Dirac Wave Functions for Solving the Molecular Matrix Dirac Equation

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Abstract

New Gaussian-transform formulas can be derived for special derivatives of Dirac wave function. Using the transform formulas, the title molecular integrals over Dirac wave functions can be derived. All molecular integral formulas can be derived for the first time. We should add the Dirac wave function to our basis set for solving the molecular matrix Dirac equation.

Keywords: Molecular Integrals, Molecular Dirac Equation, Relativistic Calculation, Dirac Wave Function, NMR Spectra.

1. Introduction

Generally speaking, the fundamental equation of the physics must be gauge invariant. The Dirac equation is the fundamental one of the relativistic quantum mechanics. Recently, Yoshizawa [1] derived the gauge invariant matrix Dirac equation with using the restricted magnetic balance [RMB] [2], as given by

$$\begin{pmatrix} \overleftrightarrow{V} & \overleftrightarrow{T_m} \\ \overleftrightarrow{T_m} & \overleftrightarrow{W_m} - \overleftrightarrow{T_m} \end{pmatrix} \begin{pmatrix} \overleftrightarrow{C_-^L} & \overleftrightarrow{C_+^L} \\ \overleftrightarrow{C_-^S} & \overleftrightarrow{C_+^S} \end{pmatrix} = \begin{pmatrix} \overleftrightarrow{S} & \overleftrightarrow{0} \\ \overleftrightarrow{0} & \frac{1}{2m_ec^2}\overleftrightarrow{T_m} \end{pmatrix} \begin{pmatrix} \overleftrightarrow{C_-^L} & \overleftrightarrow{C_+^L} \\ \overleftrightarrow{C_-^S} & \overleftrightarrow{C_+^S} \end{pmatrix} \begin{pmatrix} \overleftrightarrow{\epsilon_-} & \overleftrightarrow{0} \\ \overleftrightarrow{0} & \overleftrightarrow{\epsilon_+} \end{pmatrix} \tag{1.1}$$

where $\overleftrightarrow{C_-^L}$ is the coefficient matrix of the large component spinor for the energy matrix $\overleftrightarrow{\epsilon_-}$, $\overleftrightarrow{C_+^L}$ is that for $\overleftrightarrow{\epsilon_+}$, $\overleftrightarrow{C_-^S}$ and $\overleftrightarrow{C_+^S}$ are those for the small component spinor, $\overleftrightarrow{0}$ is the zero matrix,

$$V_{\mu\nu} = < \chi_\mu |V| \chi_\nu > \tag{1.2}$$

$$(T_m)_{\mu\nu} = \frac{1}{2m_e} < \chi_\mu |\vec{\sigma} \cdot (\vec{p} + \vec{A})\vec{\sigma} \cdot (\vec{p} + \vec{A})| \chi_\nu > \tag{1.3}$$

$$(W_m)_{\mu\nu} = \frac{1}{4m_e^2c^2} < \chi_\mu |\vec{\sigma} \cdot (\vec{p} + \vec{A})V\vec{\sigma} \cdot (\vec{p} + \vec{A})| \chi_\nu > \tag{1.4}$$

and

$$S_{\mu\nu} = < \chi_\mu | \chi_\nu > \tag{1.5}$$

in which m_e is the electron rest mass, c is the speed of light, $\vec{\sigma}$ is the Pauli spin matrices, $\vec{p} = -i\hbar\nabla$ is the momentum, and $\vec{A}$ is the vector potential due to the nuclear spin. The vector potential must be included for the invariance of the Dirac equation, as shown by Sun et al. [3]. We choose it as the Gauss-type charge density distribution [GCDD] model as given by

$$\vec{A} = \frac{Z_M e}{c^2} \frac{4}{\sqrt{\pi} r_0^3} F_1\left(\frac{r_M^2}{r_0^2}\right) \overrightarrow{\mu_M} \times \overrightarrow{r_M} \tag{1.6}$$

where $Z_M e$ is the nuclear charge of the M-th nucleus in the case that the Dirac equation is extended to the molecule, $\overrightarrow{\mu_M} = (\mu_{Mx}, \mu_{My}, \mu_{Mz})$ is the nuclear magnetic moment, $\overrightarrow{r_M} = \vec{r} - \vec{M} = (x_M, y_M, z_M)$ is the coordinate of the electron, r_0 is the scale parameter for the finite nucleus of GCDD model, and $F_m(x) = \int_0^1 dt\, t^{2m} \exp(-xt^2)$ is the molecular incomplete gamma function. We use the operator notation for all integrals.

Thus $\int_0^1 dt$ is the integral operator, which integrates the integrand followed to it. We use the atomic units

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throughout the present article ($m_e = 1$, $e = 1$, $\hbar = 1$, $4\pi\varepsilon_0 = 1$, $c = 137.035999139$). However, we describe m_e, e, and $\hbar$ explicitly, for the readers convenience when one converts the units to the natural units. Some experiment shows that the real nucleus is not the point-like one but a finite-sized [4]. However, the charge distribution in the finite nucleus is not determined. We choose the GCDD model in the present article. In the statistics, the Gauss-type distribution is called as the normal one. The gauge invariant Dirac equation has no rigorous solution. To solve it, we use a proper basis set, $\{\chi_\mu\}$.

Many researchers extend the matrix Dirac equation to the molecule [1,2,5-18]. Especially, many are for relativistic calculations of NMR spectra [1,2,14-18]. We may call the extended Dirac equation as the molecular matrix Dirac one. It is natural to add the atomic Dirac wave function to our basis set. However, all researchers use the Gaussian-type orbitals (GTOs) for their basis set, because there is no molecular integral-formula for the Dirac wave function. In previous three articles [19-21], the author derived the Gaussian-transform formulas for the Dirac wave function [19] and for its first derivative [20]. Using the transform formulas, the author derived several molecular integral-formulas over Dirac wave functions as follows: (a) He derived integral-formulas for the fundamental properties [20], as the overlap integral, $S_{\mu\nu}$, the kinetic energy one, $\frac{1}{2m_e} < \chi_\mu | p^2 | \chi_\nu >$, the nuclear attraction one, $V_{\mu\nu}$ of the point-like nucleus, $V = -\frac{Z_M e^2}{r_M}$, and of the GCDD model,

$$V = -Z_M e^2 \frac{2}{\sqrt{\pi} r_0} F_0\left(\frac{r_M^2}{r_0^2}\right) \tag{1.7}$$

the electron-repulsion one, $< \chi_\mu \chi_\kappa | V | \chi_\nu \chi_\lambda >$, of the usual one, $V = \frac{e^2}{r_{12}}$, and of the finite-sized electron, $V = \frac{2e^2}{\sqrt{\pi} r_e} F_0\left(\frac{r_{12}^2}{r_e^2}\right)$ (r_e is the classical radius of the electron), where $\chi_\mu = r_A^{-\varepsilon_A} \exp(-\zeta_A r_A)$ is the atomic Dirac wave function centered at A. Note that the Dirac wave function is singular at the position of the nucleus located at A. Therefore, the Dirac wave function cannot be written as a linear combination of GTOs.

(b) Next, he did those for relativistic kinetic energy terms given by Eq. (1.3) [21].

(c) He did that for the physical quantity [19], $< \chi_\mu | i\vec{\sigma} \cdot (\vec{p} \times V\vec{A} + \vec{A} \times V\vec{p}) | \chi_\nu >$, of the homogeneous charge density [HCDD] model,

$$V = \begin{cases} -\frac{3 Z_M e^2}{2 r_{0H}} \left(1 - \frac{1}{3}\frac{r_M^2}{r_{0H}^2}\right) & (0 \le r_M \le r_{0H}) \\ -\frac{Z_M e^2}{r_M} & (r_M > r_{0H}) \end{cases} \tag{1.8}$$

where r_{0H} is the radius of the finite-sized nucleus in the HCDD model, and of the GCDD model, V is given by Eq. (1.7). Further, the author showed that the GTO cannot describe this quantity correctly for the case of hydrogen atom [22].

In the present article, we derive the Gaussian-transform formula for a special first derivative and a special second derivative of the Dirac wave function in the next section. Using the transform formulas, we derive the quantity given by Eq. (1.4), for the GCDD model in the third section.

2. New Gaussian-Transform Formulas

First, we derive a new Gaussian-transform for the special first-derivative of the Dirac wave function. The first-derivative of the Dirac wave function can be written as

$$\nabla r_A^{-\varepsilon_A} \exp(-\zeta_A r_A) = -\vec{r_A}\left(\frac{\varepsilon_A}{r_A^{2+\varepsilon_A}} + \frac{\zeta_A}{r_A^{1+\varepsilon_A}}\right) \exp(-\zeta_A r_A) \tag{2.1}$$

The special first-derivative can be written as

$$\vec{r_A} \cdot \nabla r_A^{-\varepsilon_A} \exp(-\zeta_A r_A) = -(\varepsilon_A r_A^{-\varepsilon_A} + \zeta_A r_A^{1-\varepsilon_A}) \exp(-\zeta_A r_A) \tag{2.2}$$

The author derived the Gaussian-transform of the first term in the right-hand side of Eq. (2.2) in a previous article [19] as given by

$$-\varepsilon_A r_A^{-\varepsilon_A} \exp(-\zeta_A r_A) = \frac{-\varepsilon_A \zeta_A^{1+\varepsilon_A}}{2\sqrt{\pi}\Gamma(1+\varepsilon_A)} \int_0^\infty dS\, S^{-3/2} \exp(-S r_A^2)$$
$$\left[\frac{\zeta_A^2}{2S}\int_0^1 dt\, \frac{(1-t)^{\varepsilon_A}}{t^{4+\varepsilon_A}} - \int_0^1 dt\, \frac{(1-t)^{\varepsilon_A}}{t^{2+\varepsilon_A}}\right] exp\left[-\frac{\zeta_A^2}{4St^2}\right] \tag{2.3}$$

The Gaussian-transform of the second term in the right-hand side of Eq. (2.2) can be derived as follows: We have

$$\zeta_A r_A^{1-\varepsilon_A} \exp(-\zeta_A r_A) = \frac{\zeta_A r_A^2}{r_A^{1+\varepsilon_A}} \exp(-\zeta_A r_A) \tag{2.5}$$

We know the identity described as the formula number 3.471.3 in the Gradshteyn and Ryzhik [23] given by

$$\frac{\exp(-\beta)}{\beta^\nu} = \frac{1}{\Gamma(\nu)} \int_0^1 dt\, \frac{(1-t)^{\nu-1}}{t^{\nu+1}} exp\left(-\frac{\beta}{t}\right) \tag{2.6}$$

The author derived the Gaussian-transform of the ns-STO in a previous article [24] given by,

$$r_A^{n_A}\exp(-\zeta_A r_A)=\frac{\zeta_A^{n_A}}{2^{n_A}\sqrt{\pi}}\sum_{i_A=0}(-)^{i_A}(2i_A-1)!!\binom{n_A}{2i_A}\left(\frac{2}{\zeta_A^2}\right)^{i_A}$$
$$\int_0^\infty dS\, S^{-n_A+i_A-1/2}exp\left[-\frac{\zeta_A^2}{4S}-Sr_A^2\right] \quad (2.7)$$

Using Eq. (2.6) with $\beta=\zeta_A r_A$ and $\nu=1+\varepsilon_A$ and doing Eq. (2.7) with $\zeta_A=\frac{\zeta_A}{t}$ and $n_A=2$, we have

$$\zeta_A r_A^{1-\varepsilon_A}\exp(-\zeta_A r_A)=\frac{\zeta_A^{3+\varepsilon_A}}{4\sqrt{\pi}\Gamma(1+\varepsilon_A)}\int_0^\infty dS\, S^{-5/2}\exp(-Sr_A^2)$$
$$\left[\frac{\zeta_A^2}{2S}\int_0^1 dt\,\frac{(1-t)^{\varepsilon_A}}{t^{5+\varepsilon_A}}-3\int_0^1 dt\,\frac{(1-t)^{\varepsilon_A}}{t^{3+\varepsilon_A}}\right]exp\left[-\frac{\zeta_A^2}{4St^2}\right] \quad (2.8)$$

Substituting Eq. (2.5) and (2.8) into Eq. (2.2), we have the final formula for the special first-derivative given by

$$-\vec{r_A}\cdot\nabla r_A^{-\varepsilon_A}\exp(-\zeta_A r_A)=\frac{\zeta_A^{1+\varepsilon_A}}{2\sqrt{\pi}\Gamma(1+\varepsilon_A)}\int_0^\infty dS\exp(-Sr_A^2)$$
$$\left[\frac{\zeta_A^2}{2S}\left(\frac{\zeta_A^2}{2S}\int_0^1 dt\,\frac{(1-t)^{\varepsilon_A}}{t^{5+\varepsilon_A}}-3\int_0^1 dt\,\frac{(1-t)^{\varepsilon_A}}{t^{3+\varepsilon_A}}\right)\right.$$
$$\left.+\varepsilon_A\left(\frac{\zeta_A^2}{2S}\int_0^1 dt\,\frac{(1-t)^{\varepsilon_A}}{t^{4+\varepsilon_A}}-\int_0^1 dt\,\frac{(1-t)^{\varepsilon_A}}{t^{2+\varepsilon_A}}\right)\right]exp\left[-\frac{\zeta_A^2}{4St^2}\right] \quad (2.9)$$

Next, we derive the Gaussian-transform for the special second-derivative of the Dirac wave function given by

$$\nabla^2 r_A^{-\varepsilon_A}\exp(-\zeta_A r_A)=\left[\frac{\varepsilon_A(\varepsilon_A-1)}{r_A^{2+\varepsilon_A}}+\frac{2\zeta_A(\varepsilon_A-1)}{r_A^{1+\varepsilon_A}}+\frac{\zeta_A^2}{r_A^{\varepsilon_A}}\right]\exp(-\zeta_A r_A) \quad (2.10)$$

Using a similar derivation to that from Eq. (2.2) to (2.9), we have the final formula for the special second-derivative given by

$$\nabla^2 r_A^{-\varepsilon_A}\exp(-\zeta_A r_A)=\frac{\zeta_A^{3+\varepsilon_A}}{2\sqrt{\pi}\Gamma(1+\varepsilon_A)}\int_0^\infty dS\,S^{-3/2}\exp(-Sr_A^2)$$
$$\left[\frac{\zeta_A^2}{2S}\int_0^1 dt\,\frac{(1-t)^{\varepsilon_A}}{t^{4+\varepsilon_A}}-\int_0^1 dt\,\frac{(1-t)^{\varepsilon_A}}{t^{2+\varepsilon_A}}\right.$$
$$\left.-\frac{1-\varepsilon_A}{1+\varepsilon_A}\left(\varepsilon_A\int_0^1 dt\,\frac{(1-t)^{\varepsilon_A}}{t^{4+\varepsilon_A}}+(2+\varepsilon_A)\int_0^1 dt\,\frac{(1-t)^{\varepsilon_A}}{t^{3+\varepsilon_A}}\right)\right]exp\left[-\frac{\zeta_A^2}{4St^2}\right]$$
$$(2.11)$$

Note that, the GTO, $\exp(-Sr_A^2)$, can be converted to the object function by the integral-transform as in Eq. (2.9) and (2.11).

3. Molecular Integrals

We derive molecular integral-formulas for physical quantities given by Eq. (1.4) as follows: Using the Dirac identity [25], we have

$$(W_m)_{\mu\nu}=\frac{1}{4m_e^2c^2}<\chi_\mu|\vec{\sigma}\cdot(\vec{p}+\vec{A})V\vec{\sigma}\cdot(\vec{p}+\vec{A})|\chi_\nu>$$
$$=\frac{1}{4m_e^2c^2}<\chi_\mu|(\vec{p}+\vec{A})\cdot V(\vec{p}+\vec{A})+i\vec{\sigma}\cdot[(\vec{p}+\vec{A})\times V(\vec{p}+\vec{A})]|\chi_\nu> \quad (3.1)$$

The first physical quantity in the right-hand side of Eq. (3.1) can be written as three terms as given by

$$(\vec{p}+\vec{A})\cdot V(\vec{p}+\vec{A})=\vec{p}\cdot V\vec{p}+[\vec{p}\cdot V\vec{A}+\vec{A}\cdot V\vec{p}]+\vec{A}\cdot V\vec{A} \quad (3.2)$$

The second physical quantity can be written as two terms as given by

$$i\vec{\sigma}\cdot[(\vec{p}+\vec{A})\times V(\vec{p}+\vec{A})]=i\vec{\sigma}\cdot(\vec{p}\times V\vec{p})+i\vec{\sigma}\cdot(\vec{p}\times V\vec{A}+\vec{A}\times V\vec{p}) \quad (3.3)$$

The author already derived the molecular integral-formula over Dirac wave functions for the last term in the right-hand side of Eq. (3.3) [19]. Thus, we derive molecular integral-formulas for remaining four terms for the finite nucleus of the GCDD model in the next subsections individually.

3.1 The Term $\vec{p}\cdot V\vec{p}$

We derive molecular integral-formula for the term $\vec{p}\cdot V\vec{p}$ with the GCDD model of V, which is given by Eq. (1.7), as follows: We have

$$<\chi_{\mu A}|\vec{p}\cdot V\vec{p}|\chi_{\nu B}>=\int d\vec{r}\, r_A^{-\varepsilon_A}\exp(-\zeta_A r_A)\vec{p}\cdot V\vec{p}\, r_B^{-\varepsilon_B}\exp(-\zeta_B r_B) \quad (3.1.1)$$

The latter part of the integrand in Eq. (3.1.1) can be written as

$$\vec{p}\cdot V\vec{p}\, r_B^{-\varepsilon_B}\exp(-\zeta_B r_B)=Z_M e^2\hbar^2\nabla\frac{2}{\sqrt{\pi}r_0}F_0\left(\frac{r_M^2}{r_0^2}\right)\nabla r_B^{-\varepsilon_B}\exp(-\zeta_B r_B)$$
$$=Z_M e^2\hbar^2\left[\frac{4}{\sqrt{\pi}r_0^3}F_1\left(\frac{r_M^2}{r_0^2}\right)(-\vec{r_B})\cdot\nabla-\frac{4}{\sqrt{\pi}r_0^3}F_1\left(\frac{r_M^2}{r_0^2}\right)\overrightarrow{MB}\cdot\nabla\right.$$
$$\left.+\frac{2}{\sqrt{\pi}r_0}F_0\left(\frac{r_M^2}{r_0^2}\right)\nabla^2\right]r_B^{-\varepsilon_B}\exp(-\zeta_B r_B) \quad (3.1.2)$$

where F_m is centered at $\vec{M}=(0,0,0)$. Substituting Eq. (3.1.2) into (3.1.1) and using the Gaussian-transform formulas Eq. (2.9) and (2.11) for the resulting integral, we have

$$I=<\chi_{\mu A}|\vec{p}\cdot V\vec{p}|\chi_{\nu B}>=Z_M e^2\hbar^2\frac{\zeta_A^{1+\varepsilon_A}\zeta_B^{1+\varepsilon_B}}{4\pi\Gamma(1+\varepsilon_A)\Gamma(1+\varepsilon_B)}\int_0^\infty dS_1\int_0^\infty dS_2(S_1S_2)^{-3/2}$$
$$f_0(f_1I_1+f_2I_2+f_3I_3) \quad (3.1.3)$$

where

$$f_0=\left[\frac{\zeta_A^2}{2S_1}\int_0^1 dt_1\frac{(1-t_1)^{\varepsilon_A}}{t_1^{4+\varepsilon_A}}-\int_0^1 dt\frac{(1-t_1)^{\varepsilon_A}}{t_1^{2+\varepsilon_A}}\right]exp\left[-\frac{\zeta_A^2}{4S_1t_1^2}\right] \quad (3.1.4)$$

$$f_1=\left[\frac{\zeta_B^2}{2S_2}\left(\frac{\zeta_B^2}{2S_2}\int_0^1 dt_2\frac{(1-t_2)^{\varepsilon_B}}{t_2^{5+\varepsilon_B}}-3\int_0^1 dt_2\frac{(1-t_2)^{\varepsilon_B}}{t_2^{3+\varepsilon_B}}\right)\right.$$
$$\left.+\varepsilon_B\left(\frac{\zeta_B^2}{2S_2}\int_0^1 dt_2\frac{(1-t_2)^{\varepsilon_B}}{t_2^{4+\varepsilon_B}}-\int_0^1 dt_2\frac{(1-t_2)^{\varepsilon_B}}{t_2^{2+\varepsilon_B}}\right)\right]exp\left[-\frac{\zeta_B^2}{4S_2t_2^2}\right] \quad (3.1.5)$$

$$f_2=\left(\varepsilon_B\int_0^1 dt_2\frac{(1-t_2)^{\varepsilon_B}}{t_2^{4+\varepsilon_B}}+\int_0^1 dt_2\frac{(1-t_2)^{\varepsilon_B}}{t_2^{3+\varepsilon_B}}\right)exp\left[-\frac{\zeta_B^2}{4S_2t_2^2}\right] \quad (3.1.6)$$

$$f_3=\left[\frac{\zeta_B^2}{2S_2}\int_0^1 dt_2\frac{(1-t_2)^{\varepsilon_B}}{t_2^{4+\varepsilon_B}}-\int_0^1 dt_2\frac{(1-t_2)^{\varepsilon_B}}{t_2^{2+\varepsilon_B}}\right.$$

$$-\frac{1-\varepsilon_B}{1+\varepsilon_B}\left(\varepsilon_B\int_0^1 dt_2\frac{(1-t_2)^{\varepsilon_B}}{t_2^{4+\varepsilon_B}}+(2+\varepsilon_B)\int_0^1 dt_2\frac{(1-t_2)^{\varepsilon_B}}{t_2^{3+\varepsilon_B}}\right)\Bigg]exp\left[-\frac{\zeta_B^2}{4S_2t_2^2}\right] \quad (3.1.7)$$

$$I_1=\int d\vec{r}\,\frac{4}{\sqrt{\pi}r_0^3}F_1\left(\frac{r_M^2}{r_0^2}\right)\exp(-S_1r_A^2-S_2r_B^2) \quad (3.1.8)$$

$$I_2=\int d\vec{r}\,\frac{4\overrightarrow{MB}\cdot\overrightarrow{r_B}}{\sqrt{\pi}r_0^3}F_1\left(\frac{r_M^2}{r_0^2}\right)\exp(-S_1r_A^2-S_2r_B^2) \quad (3.1.9)$$

and

$$I_3=\int d\vec{r}\,\frac{2\zeta_B^2}{\sqrt{\pi}r_0}F_0\left(\frac{r_M^2}{r_0^2}\right)\exp(-S_1r_A^2-S_2r_B^2) \quad (3.1.10)$$

We first evaluate I_1. We use the Gaussian product rule given by

$$\exp(-S_1r_A^2-S_2r_B^2)=exp\left[-\frac{S_1S_2}{S_{12}}\overline{AB}^2-S_{12}r_P^2\right] \quad (3.1.11)$$

where $S_{12}=S_1+S_2$ and $\vec{P}=\frac{S_1}{S_{12}}\vec{A}+\frac{S_2}{S_{12}}\vec{B}$. Next, we use the Sack's formula given by [26]

$$\exp(-S_{12}r_P^2)=4\pi\exp(-S_{12}r_M^2-S_{12}\overline{MP}^2)\sum_{l=0}i_l(2S_{12}\overline{MP}r_M)$$

$$\sum_{m=-l}^{l}Y_l^m(\widehat{MP})Y_l^m(\widehat{r_M})^*, \quad (3.1.12)$$

where $i_l(x)$ is the modified spherical Bessel function of the first kind and $Y_l^m(\widehat{MP})$ is the spherical harmonics. We know that

$$i_l(x)=\frac{x^l}{(2l+1)!!}\sum_{j=0}\frac{(x^2/4)^j}{j!(l+3/2)_j} \quad (3.1.13)$$

where $(a)_j=a(a+1)\cdots(a+j-1)$ is the Pochhammer symbol. We use the Gaussian product rule again as given by

$$exp\left[-\frac{S_1S_2}{S_{12}}\overline{AB}^2\right]\exp(-S_{12}\overline{MP}^2)=\exp(-S_1\overline{MA}^2-S_2\overline{MB}^2) \quad (3.1.14)$$

Using Eq. (3.1.11), (3.1.12), and (3.1.14) for Eq. (3.1.8), we have

$$I_1=4\pi\exp(-S_1\overline{MA}^2-S_2\overline{MB}^2)I_{1a} \quad (3.1.15)$$

where

$$I_{1a}=\frac{4}{\sqrt{\pi}r_0^3}\int_0^\infty dr_M\,F_1\exp(-S_{12}r_M^2)\sum_{l=0}i_l(2S_{12}\overline{MP}r_M)$$

$$\int\widehat{r_M}\sum_{m=-l}^{l}Y_l^m(\widehat{MP})Y_l^m(\widehat{r_M})^*. \quad (3.1.16)$$

The angular part can be evaluated as in a previous article [24] given by

$$\int\widehat{r_M}\sum_{m=-l}^{l}Y_l^m(\widehat{MP})Y_l^m(\widehat{r_M})^*=\delta_{l0}. \quad (3.1.17)$$

Thus, we have

$$I_{1a}=\frac{4}{\sqrt{\pi}r_0^3}\int_0^\infty dr_M\,F_1\exp(-S_{12}r_M^2)\,i_0(2S_{12}\overline{MP}r_M)=I_{1a}^{in}+I_{1a}^{out} \quad (3.1.18)$$

where

$$I_{1a}^{in}=\frac{4}{\sqrt{\pi}r_0^3}\int_0^{R_0}dr_M\,F_1\exp(-S_{12}r_M^2)\,i_0(2S_{12}\overline{MP}r_M) \quad (3.1.19)$$

and

$$I_{1a}^{out}=\frac{4}{\sqrt{\pi}r_0^3}\int_{R_0}^\infty dr_M\,F_1\exp(-S_{12}r_M^2)\,i_0(2S_{12}\overline{MP}r_M) \quad (3.1.20)$$

in which $R_0=br_0$ $(b=7)$ separates the inner and outer part of the finite-sized nucleus of the GCDD model. We choose $b=7$ by the reason described in a previous article [19].

In the inner part, we use the power series of the $F_m(x)$ as given by

$$F_m(x)=\frac{1}{2m+1}\,{}_1F_1\left(m+\frac{1}{2};m+\frac{3}{2};-x\right)=\frac{1}{2m+1}\sum\frac{(-x)^n(m+1/2)_n}{n!(m+3/2)_n} \quad (3.1.21)$$

where ${}_1F_1(a_1;c_1;-x)$ is the confluent hypergeometric function (CHF). In the outer part, we use the asymptotic expansion of the CHF given by

$$F_m(x)=\frac{\Gamma(m+1/2)}{2x^{m+1/2}} \quad (3.1.22)$$

Using Eq. (3.1.21) for (3.1.19), we have

$$I_{1a}^{in}=\frac{4}{3\sqrt{\pi}r_0^3}\sum_{n=0}\frac{(3/2)_n(-1/r_0^2)^n}{n!(5/2)_n}\sum_{j=0}\frac{(S_{12}^2MP^2)^j}{j!(3/2)_j}\int_0^{R_0}dr_M\,r_M^{2n+2j+2}\exp(-S_{12}r_M^2 \quad (3.1.23)$$

The integral in Eq. (3.1.23) can be evaluated as given by

$$\int_0^{R_0}dr_M\,r_M^{2n+2j+2}\exp(-S_{12}r_M^2=\frac{1}{2}\int_0^{R_0^2}dx\,x^{n+j+1/2}\exp(-S_{12}x)$$

$$=\frac{1}{2}\left(\frac{1}{S_{12}}\right)^{n+j+\frac{3}{2}}\gamma\left(n+j+\frac{3}{2};S_{12}R_0^2\right)$$

$$=\frac{1}{2}R_0^{2n+2j+3}\frac{\Gamma(n+j+3/2)}{\Gamma(n+j+5/2)}\,{}_1F_1\left(n+j+\frac{3}{2};n+j+\frac{5}{2};-S_{12}R_0^2\right) \quad (3.1.24)$$

where $\gamma(\alpha;x)$ is the incomplete gamma function of the first kind, which is appeared as the formula number 8.354.1 in the Gradshteyn and Ryzhik [23] as given by

$$\gamma(\alpha,x)=\sum_{n=0}^{\infty}\frac{(-1)^nx^{\alpha+n}}{n!(\alpha+n)}=x^\alpha\frac{\Gamma(\alpha)}{\Gamma(\alpha+1)}\,{}_1F_1(\alpha;\alpha+1;-x) \quad (3.1.25)$$

Substituting Eq. (3.1.24) into (3.1.23), we have

$$I_{1a}^{in}=\frac{2b^3}{3\sqrt{\pi}}\sum_{n=0}\frac{(-b^2)^n(3/2)_n}{n!(5/2)_n}\sum_{j=0}\frac{(S_{12}^2\overline{MP}^2R_0^2)^j}{j!(3/2)_j}$$

$$\left[\frac{\Gamma(n+j+3/2)}{\Gamma(n+j+5/2)}-S_{12}R_0^2\frac{\Gamma(n+j+5/2)}{\Gamma(n+j+7/2)}+O(R_0^4)\right]$$

$$=\frac{2b^3}{3\sqrt{\pi}}\sum_{n=0}\frac{(-b^2)^n(3/2)_n}{n!(5/2)_n}\left[\frac{\Gamma(n+3/2)}{\Gamma(n+5/2)}+\left(\frac{2}{3}S_{12}^2\overline{MP}^2-S_{12}\right)R_0^2\frac{\Gamma(n+5/2)}{\Gamma(n+7/2)}+O(R_0^4)\right]$$

$$=\frac{2b^3}{3\sqrt{\pi}}\left[\frac{\Gamma(3/2)}{\Gamma(5/2)}\,{}_2F_2\left(\frac{3}{2},\frac{3}{2};\frac{5}{2},\frac{5}{2};-b^2\right)+\left(\frac{2}{3}S_{12}^2\overline{MP}^2-S_{12}\right)R_0^2\frac{\Gamma(5/2)}{\Gamma(7/2)}\,{}_1F_1\left(\frac{3}{2};\frac{7}{2};-b^2\right)\right]$$

$$+O(R_0^4) \quad (3.1.26)$$

The error term $O(R_0^4)$ is in the order of $R_0^4=0.53179747(-15)$ for the case of hydrogen, which is very small. It is easy to derive that the generalized hypergeometric function ${}_2F_2\left(\frac{3}{2},\frac{3}{2};\frac{5}{2},\frac{5}{2};-b^2\right)$ can be expressed as the integral representation given by

$${}_2F_2\left(\frac{3}{2},\frac{3}{2};\frac{5}{2},\frac{5}{2};-b^2\right)=\frac{\Gamma(5/2)\Gamma(5/2)}{\Gamma(3/2)\Gamma(3/2)}\int_0^1 du\int_0^1 dv\,\sqrt{uv}\exp(-b^2uv) \quad (3.1.27)$$

The integral in Eq. (3.1.27) has a constant value, which can be evaluated by the Gauss-Legendre quadrature (GLQ). The constant value is 0.9961218237(-2), obtained from the 4096-point GLQ. The value of the ${}_1F_1\left(\frac{3}{2};\frac{7}{2};-b^2\right)$ is also a constant. It can be evaluated by the asymptotic expansion of it from the formula number 13.5.1 of the Abramowitz and Stegun [27] as given by

$${}_1F_1\left(\frac{3}{2};\frac{7}{2};-b^2\right)=\frac{\Gamma(7/2)}{b^3}\left(1-\frac{3}{2b^2}\right) \quad (3.1.28)$$

Thus, we have

$$I_{1a}^{in}=\frac{b^3}{\sqrt{\pi}}\int_0^1 du\int_0^1 dv\,\sqrt{uv}\exp(-b^2uv)+\frac{1}{2}\left(\frac{2}{3}S_{12}^2\overline{MP}^2-S_{12}\right)\left(R_0^2-\frac{3}{2}r_0^2\right)+O(R_0^4) \quad (3.1.29)$$

Next, we evaluate I_{1a}^{out}. Using Eq. (3.1.22), we have

$$I_{1a}^{out}=\int_{R_0}^{\infty}dr_M\frac{1}{r_M}\exp(-S_{12}r_M^2)\,i_0(2S_{12}\overline{MP}r_M)$$

$$=\sum_{j=0}\frac{(S_{12}^2\overline{MP}^2)^j}{j!\,(3/2)_j}\int_{R_0}^{\infty}dr_M r_M^{2j-1}\exp(-S_{12}r_M^2)$$

$$=\frac{1}{2}\sum_{j=0}\frac{(S_{12}^2\overline{MP}^2)^j}{j!\,(3/2)_j}\int_{R_0^2}^{\infty}dx x^{j-1}\exp(-S_{12}x)$$

$$=\frac{1}{2}\int_{R_0^2}^{\infty}dx\frac{1}{x}\exp(-S_{12}x)+\frac{1}{3}S_{12}^2\overline{MP}^2\sum_{j'=0}\frac{(S_{12}^2\overline{MP}^2)^{j'}}{j'!\,(5/2)_{j'}}\int_{R_0^2}^{\infty}dx\,x^{j'}\exp(-S_{12}x)$$

$$=\frac{1}{2}\Gamma(0,S_{12}R_0^2)+\frac{1}{3}S_{12}^2\overline{MP}^2\sum_{j'=0}\frac{(S_{12}^2\overline{MP}^2)^{j'}}{j'!(5/2)_{j'}}\left(\frac{1}{S_{12}}\right)^{j'+1}\Gamma(j'+1,S_{12}R_0^2) \quad (3.1.30)$$

where $\Gamma(\alpha,x)$ is the incomplete gamma function of the second kind. We know that

$$\Gamma(0,S_{12}R_0^2)=-E_i(-S_{12}R_0^2)=-\gamma-\ln(S_{12}R_0^2)-S_{12}R_0^2+O(R_0^4) \quad (3.1.31)$$

where $\gamma=0.5772156649$ is the Euler constant and $E_i(-x)$ is the exponential integral, and it is easy to derive

$$\Gamma(j'+1,S_{12}R_0^2)=\Gamma(j'+1)-\frac{(S_{12}R_0^2)^{j'+1}}{j'+1}+O(R_0^4) \quad (3.1.32)$$

Thus, we have

$$I_{1a}^{out}=-\frac{1}{2}\gamma-\frac{1}{2}\ln(S_{12}R_0^2)+\frac{1}{3}S_{12}\overline{MP}^2\,{}_2F_2\left(1,1;2,\frac{5}{2};\,S_{12}\overline{MP}^2\right)$$

$$-\frac{1}{3}S_{12}^2\overline{MP}^2R_0^2+\frac{1}{2}S_{12}R_0^2+O(R_0^4) \quad (3.1.33)$$

Substituting Eq. (3.1.29) and (3.1.33) into (3.1.18), we have

$$I_{1a}=-\frac{1}{2}\ln(S_{12}R_0^2)+C_0+\frac{1}{3}S_{12}\overline{MP}^2\,{}_2F_2\left(1,1;2,\frac{5}{2};\,S_{12}\overline{MP}^2\right)$$

$$-\frac{1}{2}S_{12}^2\overline{MP}^2r_0^2+\frac{3}{4}S_{12}r_0^2+O(R_0^4) \quad (3.1.34)$$

where

$$C_0=\frac{b^3}{\sqrt{\pi}}\int_0^1 du\int_0^1 dv\,\sqrt{uv}\exp(-b^2uv)-\frac{1}{2}\gamma=1.639057508 \quad (3.1.35)$$

Next, we derive I_2 and I_3. Using a similar derivation from Eq. (3.1.11) to (3.1.34) for I_1, we have

$$I_2=4\pi\exp(-S_1\overline{MA}^2-S_2\overline{MB}^2)\,I_{2a} \quad (3.1.36)$$

and

$$I_3=4\pi\exp(-S_1\overline{MA}^2-S_2\overline{MB}^2)\,I_{3a} \quad (3.1.37)$$

where

$$I_{2a}=\frac{\zeta_B^2}{3}\overrightarrow{MB}\cdot$$

$$\overrightarrow{MP}\,{}_1F_1\left(1;\frac{5}{2};\,S_{12}\overline{MP}^2\right)-\frac{\zeta_B^2}{2}\overrightarrow{MB}\cdot\overrightarrow{MP}S_{12}r_0^2-\zeta_B^2\overline{MB}^2I_{1a}+O(R_0^4) \quad (3.1.38)$$

and

$$I_{3a}=\frac{1}{2}\frac{\zeta_B^2}{S_{12}}\,{}_1F_1\left(1;\frac{3}{2};\,S_{12}\overline{MP}^2\right)-\frac{1}{4}\zeta_B^2r_0^2+O(R_0^4) \quad (3.1.39)$$

Substituting Eq. (3.1.34) into (3.1.15), doing (3.1.38) into (3.1.36), doing (3.1.39) into (3.1.37), and doing these resulting equations into (3.1.3), we have

$$I=Z_Me\hbar^2\frac{\zeta_A^{1+\varepsilon_A}\zeta_B^{1+\varepsilon_B}}{\Gamma(1+\varepsilon_A)\Gamma(1+\varepsilon_B)}\int_0^{\infty}dS_1\int_0^{\infty}dS_2(S_1S_2)^{-3/2}\exp(-S_1\overline{MA}^2-S_2\overline{MB}^2)f_0$$

$$\{(f_1-f_2\zeta_B^2\overline{MB}^2)I_{1a}+f_2I_{2a}+f_3I_{3a}\}+O(R_0^4) \quad (3.1.40)$$

We evaluate the remaining integrals by the numerical integration. To do this, we first change integral variables as follows: We set $S_{12}=z$ and $\frac{S_1}{S_{12}}=w$. The Jacobian is given by

$$\frac{\partial(S_1,S_2)}{\partial(z,w)}=z \quad (3.1.41)$$

Then, we have

$$I=Z_Me\hbar^2\frac{\zeta_A^{1+\varepsilon_A}\zeta_B^{1+\varepsilon_B}}{\Gamma(1+\varepsilon_A)\Gamma(1+\varepsilon_B)}\int_0^1 dw\,[w(1-w)]^{-3/2}\int_0^{\infty}dz\,z^{-2}$$

$$exp[-wz\overline{MA}^2-(1-w)z\overline{MB}^2]f_0$$

$$\{(f_1-f_2\zeta_B^2\overline{MB}^2)I_{1a}+f_2I_{2a}+f_3I_{3a}\}+O(R_0^4) \quad (3.1.42)$$

Further, we separate integral over z as follows: $\int_0^{\infty}dz=\int_0^{a^2}dz+\int_{a^2}^{\infty}dz$ where a^2 can be chosen arbitrary. We choose $a^2=4$ here. In the first integral in the right-hand side of the above, we change integral variable from z to $u=a^2z$ and do that from z to $u=z/a^2$ in the second integral. Then we have

$$\int_0^{\infty}dz=a^2\int_0^1 du+a^2\int_0^1 du\frac{1}{u^2} \quad (3.1.43)$$

Thus, all integrals are for the interval $[0,1]$, which can be evaluated numerically by using the GLQ. Using Eq. (3.1.43), we have the final formula given by

$$I = Z_M e\hbar^2 \frac{\zeta_A^{1+\varepsilon_A}\zeta_B^{1+\varepsilon_B}}{a^2\Gamma(1+\varepsilon_A)\Gamma(1+\varepsilon_B)} \int_0^1 dw\, [w(1-w)]^{-3/2}$$

$$\left\{ \int_0^1 du\, exp[-wua^2\overline{MA}^2 - (1-w)ua^2\overline{MB}^2]\, f_0^{(1)} \right.$$

$$\left[f_1^{(1)} I_{1a}^{(1)} + f_2^{(1)} I_{2a}^{(1)} + f_3^{(1)} I_{3a}^{(1)}\right]$$

$$+ \int_0^1 du\, exp\left[-\frac{w}{u} a^2\overline{MA}^2 - \frac{1-w}{u} a^2\overline{MB}^2\right] f_0^{(2)}$$

$$\left.\left[f_1^{(2)} I_{1a}^{(2)} + f_2^{(2)} I_{2a}^{(2)} + f_3^{(2)} I_{3a}^{(2)}\right] \right\} + O(R_0^4) \tag{3.1.44}$$

where

$$f_0^{(1)} = \left[\frac{\zeta_A^2}{2wu\,a^2}\int_0^1 dt_1 \frac{(1-t_1)^{\varepsilon A}}{t_1^{4+\varepsilon A}} - \int_0^1 dt_1 \frac{(1-t_1)^{\varepsilon A}}{t_1^{2+\varepsilon A}}\right] exp\left[-\frac{\zeta_A^2}{4wu\,a^2 t_1^2}\right] \tag{3.1.45}$$

$$f_1^{(1)} = \left[\ \frac{\zeta_B^2}{2(1-w)ua^2}\left(\frac{\zeta_B^2}{2(1-w)ua^2}\int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon_B}}{t_2^{5+\varepsilon_B}} - 3\int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon_B}}{t_2^{3+\varepsilon_B}}\right)\right.$$

$$\left. +\varepsilon_B\left(\frac{u\zeta_B^2}{2(1-w)a^2}\int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon B}}{t_2^{4+\varepsilon B}} - \int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon B}}{t_2^{2+\varepsilon B}}\right)\ \right] exp\left[-\frac{u\zeta_B^2}{4(1-w)a^2 t_2^2}\right] \tag{3.1.46}$$

$$f_2^{(1)} = \left(\varepsilon_B \int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon B}}{t_2^{4+\varepsilon B}} + \int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon B}}{t_2^{3+\varepsilon B}}\right) exp\left[-\frac{\zeta_B^2}{4(1-w)ua^2 t_2^2}\right] \tag{3.1.47}$$

$$f_3^{(1)} = \left[\frac{\zeta_B^2}{2(1-w)ua^2}\int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon_B}}{t_2^{4+\varepsilon_B}} - \int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon_B}}{t_2^{2+\varepsilon_B}}\right.$$

$$\left. -\frac{1-\varepsilon_B}{1+\varepsilon_B}\left(\varepsilon_B \int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon B}}{t_2^{4+\varepsilon B}} + (2+\varepsilon_B)\int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon B}}{t_2^{3+\varepsilon B}}\right)\right] exp\left[-\frac{\zeta_B^2}{4(1-w)ua^2 t_2^2}\right] \tag{3.1.48}$$

$$I_{1a}^{(1)} = -\frac{1}{2u^2}\ln(ua^2R_0^2) + \frac{C_0}{u^2} + \frac{1}{3u}a^2 x_0\, {}_2F_2\left(1,1;2,\frac{5}{2};\ ua^2x_0\right)$$

$$-\frac{1}{2u^2}a^4x_0^2r_0^2 + \frac{3a^2}{4u}r_0^2 \tag{3.1.49}$$

$$I_{2a}^{(1)} = \frac{\zeta_B^2}{3}\frac{y_0}{u^2}\, {}_1F_1\left(1;\ \frac{5}{2};\ ua^2x_0\right) - \frac{\zeta_B^2}{2}\frac{a^2y_0}{u}r_0^2 - \zeta_B^2\overline{MB}^2 I_{1a}^{(1)} \tag{3.1.50}$$

$$I_{3a}^{(1)} = \frac{1}{2}\frac{\zeta_B^2}{u^3a^2}\ {}_1F_1\left(1;\ \frac{3}{2};\ ua^2x_0\right) - \frac{1}{4u^2}\zeta_B^2 r_0^2 \tag{3.1.51}$$

$$f_0^{(2)} = \left[\frac{u\zeta_A^2}{2wa^2}\int_0^1 dt_1 \frac{(1-t_1)^{\varepsilon A}}{t_1^{4+\varepsilon A}} - \int_0^1 dt_1 \frac{(1-t_1)^{\varepsilon A}}{t_1^{2+\varepsilon A}}\right] exp\left[-\frac{u\zeta_A^2}{4wa^2t_1^2}\right] \tag{3.1.52}$$

$$f_1^{(2)} = \left[\ \frac{u\zeta_B^2}{2(1-w)a^2}\left(\frac{\zeta_B^2}{2(1-w)ua^2}\int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon_B}}{t_2^{5+\varepsilon_B}} - 3\int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon_B}}{t_2^{3+\varepsilon_B}}\right)\right.$$

$$\left. +\varepsilon_B\left(\frac{\zeta_B^2}{2(1-w)ua^2}\int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon B}}{t_2^{4+\varepsilon B}} - \int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon B}}{t_2^{2+\varepsilon B}}\right)\ \right] exp\left[-\frac{\zeta_B^2}{4(1-w)ua^2t_2^2}\right] \tag{3.1.53}$$

$$f_2^{(2)} = \left(\varepsilon_B \int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon B}}{t_2^{4+\varepsilon B}} + \int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon B}}{t_2^{3+\varepsilon B}}\right) exp\left[-\frac{u\zeta_B^2}{4(1-w)a^2t_2^2}\right] \tag{3.1.54}$$

$$f_3^{(2)} = \left[\frac{u\zeta_B^2}{2(1-w)a^2}\int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon_B}}{t_2^{4+\varepsilon_B}} - \int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon_B}}{t_2^{2+\varepsilon_B}}\right.$$

$$\left. -\frac{1-\varepsilon_B}{1+\varepsilon_B}\left(\varepsilon_B \int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon B}}{t_2^{4+\varepsilon B}} + (2+\varepsilon_B)\int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon B}}{t_2^{3+\varepsilon B}}\right)\right] exp\left[-\frac{u\zeta_B^2}{4(1-w)a^2t_2^2}\right] \tag{3.1.55}$$

$$I_{1a}^{(2)} = -\frac{1}{2}\ln\left(\frac{a^2}{u}R_0^2\right) + C_0 + \frac{1}{3u}a^2x_0\, {}_2F_2\left(1,1;2,\frac{5}{2};\ \frac{a^2}{u}x_0\right)$$

$$-\frac{1}{2}a^4x_0^2r_0^2 + \frac{3a^2}{4u}r_0^2 \tag{3.1.56}$$

$$I_{2a}^{(2)} = \frac{\zeta_B^2}{3}y_0\, {}_1F_1\left(1;\ \frac{5}{2};\ \frac{a^2}{u}x_0\right) - \frac{\zeta_B^2}{2}\frac{a^2y_0}{u}r_0^2 - \zeta_B^2\overline{MB}^2 I_{1a}^{(2)} \tag{3.1.57}$$

$$I_{3a}^{(2)} = \frac{u}{2}\frac{\zeta_B^2}{a^2}\, {}_1F_1\left(1;\ \frac{3}{2};\ \frac{a^2}{u}x_0\right) - \frac{1}{4}\zeta_B^2 r_0^2 \tag{3.1.58}$$

$$x_0 = w^2\overline{MA}^2 + (1-w)^2\overline{MB}^2 + 2w(1-w)\overrightarrow{MA}\cdot\overrightarrow{MB} \tag{3.1.59}$$

and

$$y_0 = w\overrightarrow{MA}\cdot\overrightarrow{MB} + (1-w)\overline{MB}^2. \tag{3.1.60}$$

Using the 128-point GLQ, we have the value of I with 8 significant-figure precision. We obtain $I = 0.21580602\, e\hbar^2$ for the case of three hydrogen atoms located at $\vec{M} = (0,0,0)$, $\vec{A} = (-\frac{\sqrt{8}}{3}, -\sqrt{\frac{8}{3}}, \frac{2}{3})$, and $\vec{B} = (-\frac{\sqrt{8}}{3}, \sqrt{\frac{8}{3}}, \frac{2}{3})$.

3.2 The Term $\vec{A}\cdot V\vec{A}$

We evaluate the molecular integral-formula over Dirac wave functions for the term $\vec{A}\cdot V\vec{A}$ with potentials of the finite nucleus for the GCDD model as follows: The $\vec{A}$ is given by Eq. (1.6). We have

$$< \chi_{\mu A}|\vec{A}\cdot V\vec{A}|\chi_{\nu B} >= -\frac{Z_M^3 e^4}{c^4}\sum_{\xi,\eta}\mu_{M\xi}\mu_{M\eta}I_{\xi\eta}\quad \xi,\eta \in (x,y,z) \tag{3.2.1}$$

where

$$I_{\xi\eta} = \frac{32}{\pi^{3/2}r_0^7}\int d\vec{r}\, F_0F_1F_1(\delta_{\xi\eta}r_M^2 - \xi_M\eta_M)r_A^{-\varepsilon_A}r_B^{-\varepsilon_B}\exp(-\zeta_Ar_A - \zeta_Br_B) \tag{3.2.2}$$

We first derive

$$I_{zz} = \frac{32}{\pi^{3/2}r_0^7}\int d\vec{r}\, F_0F_1F_1(r_M^2 - z_M^2)r_A^{-\varepsilon_A}r_B^{-\varepsilon_B}\exp(-\zeta_Ar_A - \zeta_Br_B) \tag{3.2.3}$$

We use the Gaussian-transform for the Dirac wave function centered at A, as given by

$$r_A^{-\varepsilon_A}\exp(-\zeta_Ar_A) = \frac{\zeta_A^{1+\varepsilon_A}}{2\sqrt{\pi}\Gamma(1+\varepsilon_A)}\int_0^\infty dS_1\, S_1^{-3/2}\exp(-S_1r_A^2)\, f_0 \tag{3.2.4}$$

where f_0 is given by Eq. (3.1.4). We use also that centered at B and have

$$I_{zz} = \frac{\zeta_A^{1+\varepsilon_A}\zeta_B^{1+\varepsilon_B}}{4\pi\Gamma(1+\varepsilon_A)\Gamma(1+\varepsilon_B)}\int_0^\infty dS_1\int_0^\infty dS_2\,(S_1S_2)^{-3/2}f_0f_{0B}I_1^{zz} \tag{3.2.5}$$

where

$$f_{0B} = \left[\frac{\zeta_B^2}{2S_2}\int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon B}}{t_2^{4+\varepsilon B}} - \int_0^1 dt_2 \frac{(1-t_2)^{\varepsilon B}}{t_2^{2+\varepsilon B}}\right] exp\left[-\frac{\zeta_B^2}{4S_2t_2^2}\right] \tag{3.2.6}$$

and

$$I_1^{zz} = \frac{32}{\pi^{3/2}r_0^7}\int d\vec{r}\ F_0F_1F_1(r_M^2 - z_M^2)\exp(-S_1r_A^2 - S_2r_B^2) \tag{3.2.7}$$

We know that $r_M^2 - z_M^2 = \frac{2}{3}r_M^2 - \frac{2}{3}S_{20}(\overrightarrow{r_M})$. Then, we have

$$I_1^{zz} = I_2^{zz} + I_3^{zz} \tag{3.2.8}$$

where

$$I_2^{zz} = \frac{64}{3\pi^{3/2} r_0^7} \int d\vec{r}\; r_M^2 F_0 F_1 F_1 \exp(-S_1 r_A^2 - S_2 r_B^2) \tag{3.2.9}$$

and

$$I_3^{zz} = \frac{-64}{3\pi^{3/2} r_0^7} \int d\vec{r}\; F_0 F_1 F_1 \exp(-S_1 r_A^2 - S_2 r_B^2) S_{20}(\overrightarrow{r_M}) \tag{3.2.10}$$

Using the Gaussian-product rule, Eq. (3.1.11), the Sack's formula, Eq. (3.1.12), and the Gaussian-product rule again, Eq. (3.1.14), we have

$$I_2^{zz} = 4\pi \exp(-S_1 \overline{MA}^2 - S_2 \overline{MB}^2) I_{2a}^{zz}, \tag{3.2.11}$$

and

$$I_3^{zz} = 4\pi \exp(-S_1 \overline{MA}^2 - S_2 \overline{MB}^2) I_{3a}^{zz}, \tag{3.2.12}$$

where

$$I_{2a}^{zz} = \frac{64}{3\pi^{3/2} r_0^7} \int_0^\infty dr_M\, r_M^4 F_0 F_1 F_1 \exp(-S_{12} r_M^2) \sum_{l=0} i_l(2S_{12}\overline{MP} r_M)$$

$$\int \widehat{r_M} \sum_{m=-l}^{l} Y_l^m(\widehat{MP})\, Y_l^m(\widehat{r_M})^*, \tag{3.2.13}$$

and

$$I_{3a}^{zz} = \frac{-64}{3\pi^{3/2} r_0^7} \int_0^\infty dr_M\, r_M^2 F_0 F_1 F_1 \exp(-S_{12} r_M^2) \sum_{l=0} i_l(2S_{12}\overline{MP} r_M)$$

$$\int \widehat{r_M} \sum_{m=-l}^{l} Y_l^m(\widehat{MP})\, Y_l^m(\widehat{r_M})^* S_{20}(\overrightarrow{r_M}). \tag{3.2.14}$$

The angular part can be evaluated by using Eq. (3.1.17) and as in a previous article [24] as given by

$$\int \widehat{r_M} \sum_{m=-l}^{l} Y_l^m(\widehat{MP})\, Y_l^m(\widehat{r_M})^* S_{20}(\overrightarrow{r_M}) = r_M^2\, \delta_{l2} \frac{S_{20}(\overrightarrow{MP})}{\overline{MP}^2} \tag{3.2.15}$$

Thus, we have

$$I_{2a}^{zz} = \frac{64}{3\pi^{3/2} r_0^7} \int_0^\infty dr_M\, r_M^4 F_0 F_1 F_1 \exp(-S_{12} r_M^2)\, i_0(2S_{12}\overline{MP} r_M) \tag{3.2.16}$$

and

$$I_{3a}^{zz} = \frac{-64}{3\pi^{3/2} r_0^7} \frac{S_{20}(\overrightarrow{MP})}{\overline{MP}^2} \int_0^\infty dr_M\, r_M^4 F_0 F_1 F_1 \exp(-S_{12} r_M^2)\, i_2(2S_{12}\overline{MP} r_M) \tag{3.2.17}$$

We evaluate I_{2a}^{zz} as follows: We have

$$I_{2a}^{zz} = I_{2a}^{zzin} + I_{2a}^{zzout} \tag{3.2.18}$$

where

$$I_{2a}^{zzin} = \frac{64}{3\pi^{3/2} r_0^7} \int_0^{R_0} dr_M\, r_M^4 F_0 F_1 F_1 \exp(-S_{12} r_M^2)\, i_0(2S_{12}\overline{MP} r_M) \tag{3.2.19}$$

and

$$I_{2a}^{zzout} = \frac{64}{3\pi^{3/2} r_0^7} \int_{R_0}^\infty dr_M\, r_M^4 F_0 F_1 F_1 \exp(-S_{12} r_M^2)\, i_0(2S_{12}\overline{MP} r_M) \tag{3.2.20}$$

In order to evaluate I_{2a}^{zzin}, we use Eq. (3.1.13) and (3.1.21) and have

$$I_{2a}^{zzin} = \frac{64}{27\pi^{3/2} r_0^7} \sum_{j=0} \frac{(S_{12}^2 \overline{MP}^2)^j}{j!\,(3/2)_j}$$

$$\sum_{n_1 n_2 n_3=0} \frac{(-1/r_0^2)^{n_1+n_2+n_3} (3/2)_{n_1} (3/2)_{n_2} (1/2)_{n_3}}{n_1! n_2! n_3! (5/2)_{n_1} (5/2)_{n_2} (3/2)_{n_3}} I_{2b}^{zzin} \tag{3.2.21}$$

where

$$I_{2b}^{zzin} = \int_0^{R_0} dr_M\; r_M^{2(j+n_{123})+4} \exp(-S_{12} r_M^2)$$

$$= \frac{1}{2}\int_0^{R_0^2} dx\; x^{j+n_{123}+3/2} \exp(-S_{12}x) = \frac{1}{2}\left(\frac{1}{S_{12}}\right)^{j+n_{123}} \gamma(j+n_{123};\, S_{12}R_0^2)$$

$$= \frac{1}{2}\left(\frac{1}{S_{12}}\right)^{j+n_{123}+5/2} (S_{12}R_0^2)^{j+n_{123}+5/2} \frac{\Gamma(j+n_{123}+5/2)}{\Gamma(j+n_{123}+7/2)}$$

$${}_1F_1\left(j+n_{123}+\frac{5}{2};\, j+n_{123}+\frac{7}{2};\, -S_{12}R_0^2\right)$$

$$= \frac{1}{2}(R_0^2)^{j+n_{123}+5/2} \frac{\Gamma(j+n_{123}+5/2)}{\Gamma(j+n_{123}+7/2)}\, {}_1F_1\left(j+n_{123}+\frac{5}{2};\, j+n_{123}+\frac{7}{2};\, -S_{12}R_0^2\right) \tag{3.2.22}$$

where $n_{123} = n_1 + n_2 + n_3$. Substituting Eq. (3.2.22) into (3.2.21), we have

$$I_{2a}^{zzin} = \frac{64}{27\pi^{3/2} r_0^7} \sum_{j=0} \frac{(S_{12}^2 \overline{MP}^2)^j}{j!(3/2)_j}$$

$$\sum_{n_1 n_2 n_3=0} \frac{(-b^2)^{n_{123}} (3/2)_{n_1} (3/2)_{n_2} (1/2)_{n_3}}{n_1! n_2! n_3! (5/2)_{n_1} (5/2)_{n_2} (3/2)_{n_3}}$$

$$\frac{\Gamma(j+n_{123}+5/2)}{\Gamma(j+n_{123}+7/2)}\, {}_1F_1\left(j+n_{123}+\frac{5}{2};\, j+n_{123}+\frac{7}{2};\, -S_{12}R_0^2\right)$$

$$= \frac{32\, b^5}{27\pi^{3/2} r_0^2}\Big[\; S_{A0} + \left(\frac{2}{3}S_{12}^2\overline{MP}^2 - S_{12}\right) R_0^2 S_{A1}$$

$$+ \left(\frac{4}{15}S_{12}^4\overline{MP}^4 - \frac{2}{3}S_{12}^3\overline{MP}^2 + \frac{1}{2}S_{12}^2\right) R_0^4 S_{A2} + O(R_0^6) \tag{3.2.23}$$

where

$$S_{A0} = \sum_{n_1 n_2 n_3=0} \frac{(-b^2)^{n_{123}} (3/2)_{n_1} (3/2)_{n_2} (1/2)_{n_3}}{n_1! n_2! n_3! (5/2)_{n_1} (5/2)_{n_2} (3/2)_{n_3}} \frac{\Gamma(n_{123}+5/2)}{\Gamma(n_{123}+7/2)} \tag{3.2.24}$$

$$S_{A1} = \sum_{n_1 n_2 n_3=0} \frac{(-b^2)^{n_{123}} (3/2)_{n_1} (3/2)_{n_2} (1/2)_{n_3}}{n_1! n_2! n_3! (5/2)_{n_1} (5/2)_{n_2} (3/2)_{n_3}} \frac{\Gamma(n_{123}+7/2)}{\Gamma(n_{123}+9/2)} \tag{3.2.25}$$

and

$$S_{A2} = \sum_{n_1 n_2 n_3=0} \frac{(-b^2)^{n_{123}} (3/2)_{n_1} (3/2)_{n_2} (1/2)_{n_3}}{n_1! n_2! n_3! (5/2)_{n_1} (5/2)_{n_2} (3/2)_{n_3}} \frac{\Gamma(n_{123}+9/2)}{\Gamma(n_{123}+11/2)} \tag{3.2.26}$$

Summations, Eq. (3.2.24), (3.2.25) and (3.2.26), can be calculated in Appendix A.

Substituting Eq. (a.33), (a.35), and (a.41), into (3.2.23), we have

$$I_{2a}^{zzin} = \frac{2}{3r_0^2} - \frac{1}{3R_0^2} - \frac{4}{3\pi r_0^2} - \frac{1}{\pi r_0^2}(C_{A0a} - C_{A0b} - C_{A0c} + C_{A0d})$$

$$+ \left(\frac{2}{3}S_{12}^2\overline{MP}^2 - S_{12}\right)\left[\frac{b^3}{3\sqrt{\pi}} C_{A1a} - \frac{8}{3\sqrt{\pi}} C_{A1b} - \frac{5}{2\pi}(C_{A1c} - C_{A1d})\right]$$

$$+ \left(\frac{4}{15}S_{12}^4\overline{MP}^4 - \frac{2}{3}S_{12}^3\overline{MP}^2 + \frac{1}{2}S_{12}^2\right) \tag{3.2.27}$$

$$\left[\; \frac{R_0^2}{3} - \frac{r_0^2}{2} - \frac{2r_0^2}{3\pi} - \frac{35 r_0^2}{4\pi}(C_{A2c} - C_{A2d} - C_{A2e} + C_{A2f}) \;\right] + O(R_0^4)$$

Next, we evaluate I_{2a}^{zzout}. For the outer part of the finite nucleus, we use the asymptotic expansion of the molecular incomplete gamma function given by Eq. (3.1.22). Substituting Eq. (3.1.22) into (3.2.20), we have

$$I_{2a}^{zzout} = \frac{2}{3}\int_{R_0}^\infty dr_M \frac{1}{r_M^3} \exp(-S_{12} r_M^2)\, i_0(2S_{12}\overline{MP} r_M) = \frac{2}{3}\sum_{j=0} \frac{(S_{12}^2\overline{MP}^2)^j}{j!(3/2)_j} I_{2b}^{zzout} \tag{3.2.28}$$

where

$$I_{2b}^{zzout}=\int_{R_0}^{\infty}dr_M\, r_M^{2j-3}\exp(-S_{12}r_M^2)=\frac{1}{2}\int_{R_0^2}^{\infty}dx\, x^{j-2}\exp(-S_{12}x)$$

$$=\frac{\delta_{j0}}{2}\int_{R_0^2}^{\infty}dx\,\frac{1}{x^2}\exp(-S_{12}x)+\frac{\delta_{j1}}{2}\int_{R_0^2}^{\infty}dx\,\frac{1}{x}\exp(-S_{12}x)$$

$$+\frac{1-\delta_{j0}-\delta_{j1}}{2}\int_{R_0^2}^{\infty}dx\, x^{j-2}\exp(-S_{12}x) \quad (3.2.29)$$

Substituting Eq. (3.2.26) into (3.2.25), we have

$$I_{2a}^{zzout}=\frac{S_{12}}{3}\Gamma(-1,S_{12}R_0^2)+\frac{2}{9}S_{12}^2\overline{MP}^2\Gamma(0,S_{12}R_0^2)$$

$$+\frac{4}{45}S_{12}^4\overline{MP}^4\sum_{j'=0}\frac{(S_{12}^2\overline{MP}^2)^{j'}}{(3)_{j'}(7/2)_{j'}}\left(\frac{1}{S_{12}}\right)^{j'+1}\Gamma(j'+1,S_{12}R_0^2) \quad (3.2.30)$$

We use the formula number 8.352.8 of Gradshteyn and Ryzhik [23] as given by

$$\Gamma(-n+k,x)=\frac{(-1)^{n-k}}{(n-k)!}\left[\Gamma(0,x)-\exp(-x)\sum_{m=0}^{n-k-1}(-1)^m\frac{m!}{x^{m+1}}\right] \quad (3.2.31)$$

Thus, we have

$$\Gamma(-1,S_{12}R_0^2)=E_i(-S_{12}R_0^2)+\frac{\exp(-S_{12}R_0^2)}{S_{12}R_0^2}$$

$$-\frac{R_0^2}{3}\left(\frac{4}{15}S_{12}^4\overline{MP}^4-\frac{2}{3}S_{12}^3\overline{MP}^2+\frac{1}{2}S_{12}^2\right)+O(R_0^4)$$

$$=\gamma+\ln(S_{12}R_0^2)-S_{12}R_0^2+\frac{1}{S_{12}R_0^2}-1+\frac{1}{2}S_{12}R_0^2+O(R_0^4) \quad (3.2.32)$$

Substituting Eq. (3.2.32), (3.1.31), and (3.1.32) into (3.2.30), we have

$$I_{2a}^{zzout}=\frac{1}{3R_0^2}-\frac{1}{3}\left(\frac{2}{3}S_{12}^2\overline{MP}^2-S_{12}\right)[\gamma+\ln(S_{12}R_0^2)]$$

$$-\frac{S_{12}}{3}+\frac{4}{45}S_{12}^3\overline{MP}^4\,{}_2F_2\left(1,1;3,\frac{7}{2};\ S_{12}\overline{MP}^2\right) \quad (3.2.33)$$

$$-\frac{R_0^2}{3}\left(\frac{4}{15}S_{12}^4\overline{MP}^4-\frac{2}{3}S_{12}^3\overline{MP}^2+\frac{1}{2}S_{12}^2\right)+O(R_0^4)$$

Substituting Eq. (3.2.27) and (3.2.33) into (3.2.18), we have

$$I_{2a}^{zz}=\frac{C_{A0}}{r_0^2}+\frac{1}{3}\left(\frac{2}{3}S_{12}^2\overline{MP}^2-S_{12}\right)$$

$$\left[C_{A1}+\ln(S_{12}R_0^2)-\frac{S_{12}}{3}+\frac{4}{45}S_{12}^3\overline{MP}^4\,{}_2F_2\left(1,1;3,\frac{7}{2};\ S_{12}\overline{MP}^2\right)\right] \quad (3.2.34)$$

where

$$C_{A0}=\frac{2}{3}-\frac{4}{3\pi}-\frac{1}{\pi}(C_{A0a}-C_{A0b}-C_{A0c}+C_{A0d})=0.2222222222 \quad (3.2.35)$$

$$C_{A1}=\gamma-\frac{2b^3}{\sqrt{\pi}}C_{A1a}+\frac{8}{\sqrt{\pi}}C_{A1b}-\frac{15}{2\pi}(C_{A1c}-C_{A1d})=-2.287894210 \quad (3.2.36)$$

and

$$C_{A2}=-\frac{1}{2}-\frac{2}{3\pi}-\frac{35}{4\pi}(C_{A2c}-C_{A2d}-C_{A2e}+C_{A2f})=-0.7360218971 \quad (3.2.37)$$

Next, we evaluate I_{3a}^{zz} as follows: We have

$$I_{3a}^{zz}=I_{3a}^{zzin}+I_{3a}^{zzout} \quad (3.2.38)$$

where

$$I_{3a}^{zzin}=\frac{-64}{3\pi^{3/2}r_0^7}\frac{S_{20}(\overrightarrow{MP})}{\overline{MP}^2}\int_0^{R_0}dr_M\, r_M^4F_0F_1F_1\exp(-S_{12}r_M^2)\,i_2(2S_{12}\overline{MP}r_M) \quad (3.2.39)$$

and

$$I_{3a}^{zzout}=\frac{-64}{3\pi^{3/2}r_0^7}\frac{S_{20}(\overrightarrow{MP})}{\overline{MP}^2}\int_{R_0}^{\infty}dr_M\, r_M^4F_0F_1F_1\exp(-S_{12}r_M^2)\,i_2(2S_{12}\overline{MP}r_M) \quad (3.2.40)$$

With a similar derivation to that for I_{2a}^{zzin}, we have

$$I_{3a}^{zzin}=S_{12}^2S_{20}(\overrightarrow{MP})\Bigg\{-\frac{8b^3}{45\sqrt{\pi}}\int_0^1du\int_0^1dv\,\sqrt{uv}\exp(-b^2uv)$$

$$+\frac{32}{45\sqrt{\pi}}\int_0^1du\int_0^1dv\,\frac{\sqrt{uv}}{(1+uv)^3}+\frac{2}{3\pi}\int_0^1ds\int_0^1du\int_0^1dv\,\frac{\sqrt{suv}}{(1+s+uv)^{7/2}}$$

$$-\frac{2}{3\pi}\int_0^1ds\int_0^1du\int_0^1dv\,\frac{s^2\sqrt{uv}}{(1+s+suv)^{7/2}}$$

$$+\left(\frac{2}{7}S_{12}^2\overline{MP}^2-S_{12}\right)\Bigg[-\frac{4R_0^2}{45}+\frac{2r_0^2}{15}+\frac{8r_0^2}{45\pi}$$

$$+\frac{7r_0^2}{3\pi}\int_0^1ds\int_0^1du\,\frac{\sqrt{su}}{(1+s+u)^{9/2}}-\frac{7r_0^2}{3\pi}\int_0^1ds\int_0^1du\,\frac{\sqrt{s}u^{3/2}}{(1+s+u)^{9/2}}$$

$$-\frac{7r_0^2}{3\pi}\int_0^1ds\int_0^1du\,\frac{s^3\sqrt{u}}{(1+s+su)^{9/2}}+\frac{7r_0^2}{3\pi}\int_0^1ds\int_0^1du\,\frac{s^3u^{3/2}}{(1+s+su)^{9/2}}\Bigg]\Bigg\}$$

$$+O(R_0^4) \quad (3.2.41)$$

All integrals in the above Eq. (3.2.41) are constants as given by Eq. (a.36), (a.37), (a.46), (a.47), (a.48), and (a.49). Substituting these constants into Eq. (3.2.41), we have

$$I_{3a}^{zzin}=S_{12}^2S_{20}(\overrightarrow{MP})\Bigg\{\frac{-8b^3}{45\sqrt{\pi}}C_{A1a}+\frac{32}{45\sqrt{\pi}}C_{A1b}+\frac{2}{3\pi}(C_{A1c}-C_{A1d})$$

$$+\left(\frac{2}{7}S_{12}^2\overline{MP}^2-S_{12}\right)\Bigg[-\frac{4R_0^2}{45}+\frac{2r_0^2}{15}+\frac{8r_0^2}{45\pi}$$

$$+\frac{7r_0^2}{3\pi}(C_{A2c}-C_{A2d}-C_{A2e}+C_{A2f})\Bigg]\Bigg\}+O(R_0^4) \quad (3.2.42)$$

For the term I_{3a}^{zzout}, with a similar derivation to that for I_{2a}^{zzout}, we have

$$I_{3a}^{zzout}=S_{12}^2S_{20}(\overrightarrow{MP})\Bigg\{\frac{4}{45}[\gamma+\ln(S_{12}R_0^2)]-\frac{8}{315}S_{12}\overline{MP}^2\,{}_2F_2\left(1,1;2,\frac{9}{2};\ S_{12}\overline{MP}^2\right)$$

$$+\frac{4R_0^2}{45}\left(\frac{2}{7}S_{12}^2\overline{MP}^2-S_{12}\right)+O(R_0^4)\Bigg\} \quad (3.2.43)$$

Substituting Eq. (3.2.42) and (3.2.43) into (3.2.38), we have

$$I_{3a}^{zz}=S_{12}^2S_{20}(\overrightarrow{MP})\Bigg\{\frac{4}{45}[\ln(S_{12}R_0^2)+C_{A1}]-\frac{8}{315}S_{12}\overline{MP}^2\,{}_2F_2\left(1,1;2,\frac{9}{2};\ S_{12}\overline{MP}^2\right)$$

$$+\left(\frac{2}{7}S_{12}^2\overline{MP}^2-S_{12}\right)r_0^2C_{A3}\Bigg\}+O(R_0^4) \quad (3.2.44)$$

where

$$C_{A3}=\frac{2}{15}+\frac{8}{45\pi}+\frac{7}{3\pi}(C_{A2c}-C_{A2d}-C_{A2e}+C_{A2f})=0.1962725059 \quad (3.2.45)$$

Substituting Eq. (3.2.34) into (3.2.11), doing (3.2.44) into (3.2.12), and doing these resulting equations into (3.2.8), we have

$$I_1^{zz}=4\pi\Bigg\{\frac{C_{A0}}{r_0^2}+\left(\frac{4}{45}S_{12}^2S_{20}(\overrightarrow{MP})+\frac{2}{9}S_{12}^2\overline{MP}^2-\frac{1}{3}S_{12}\right)[\ln(S_{12}R_0^2)+C_{A1}]$$

$$-\frac{S_{12}}{3}+\frac{4}{45}S_{12}^3\overline{MP}^4\,{}_2F_2\left(1,1;3,\frac{7}{2};\;S_{12}\overline{MP}^2\right)$$

$$-\frac{8}{315}S_{12}^3\overline{MP}^2S_{20}(\overrightarrow{MP})\,{}_2F_2\left(1,1;2,\frac{9}{2};\;S_{12}\overline{MP}^2\right)$$

$$+\left(\frac{4}{15}S_{12}^4\overline{MP}^4-\frac{2}{3}S_{12}^3\overline{MP}^2+\frac{1}{2}S_{12}^2\right)r_0^2C_{A2}$$

$$+\left(\tfrac{2}{7}S_{12}^2\overline{MP}^2-S_{12}\right)r_0^2C_{A3}\quad\Big\}+O(R_0^4)\qquad(3.2.46)$$

Substituting Eq. (3.2.46) into (3.2.5), we have

$$I_{zz}=\frac{\zeta_A^{1+\varepsilon_A}\zeta_B^{1+\varepsilon_B}}{\Gamma(1+\varepsilon_A)\Gamma(1+\varepsilon_B)}\int_0^\infty dS_1\int_0^\infty dS_2\,(S_1S_2)^{-3/2}f_0f_{0B}$$

$$\Big\{\ \frac{C_{A0}}{r_0^2}+\left(\frac{4}{45}S_{12}^2S_{20}(\overrightarrow{MP})+\frac{2}{9}S_{12}^2\overline{MP}^2-\frac{1}{3}S_{12}\right)[\ln(S_{12}R_0^2)+C_{A1}]$$

$$-\frac{S_{12}}{3}+\frac{4}{45}S_{12}^3\overline{MP}^4\,{}_2F_2\left(1,1;3,\frac{7}{2};\;S_{12}\overline{MP}^2\right)$$

$$-\frac{8}{315}S_{12}^3\overline{MP}^2S_{20}(\overrightarrow{MP})\,{}_2F_2\left(1,1;2,\frac{9}{2};\;S_{12}\overline{MP}^2\right)$$

$$+\left(\frac{4}{15}S_{12}^4\overline{MP}^4-\frac{2}{3}S_{12}^3\overline{MP}^2+\frac{1}{2}S_{12}^2\right)r_0^2C_{A2}$$

$$+\left(\frac{2}{7}S_{12}^2\overline{MP}^2-S_{12}\right)r_0^2C_{A3}\quad\Big\}+O(R_0^4)\qquad(3.2.47)$$

We evaluate the remaining integrals by the numerical integration. To do this, we first change integral variables as follows: We set $S_{12}=z$ and $\frac{S_1}{S}=w$. The Jacobian is given by Eq. (3.1.41). Further, we separate integral over z as is same as for Eq. (3.1.43). Then, we have the final formula given by

$$I_{zz}=\frac{\zeta_A^{1+\varepsilon_A}\zeta_B^{1+\varepsilon_B}}{\Gamma(1+\varepsilon_A)\Gamma(1+\varepsilon_B)a^2}\int_0^1 dw\,[w(1-w)]^{-3/2}$$

$$\Big\{\ \int_0^1 du\,exp[-wua^2\overline{MA}^2-(1-w)ua^2\overline{MB}^2]f_0^{(1)}f_{0B}^{(1)}$$

$$\Big[\ \frac{C_{A0}}{u^2r_0^2}+\left(\frac{4}{45}a^4y_0-\frac{2}{9}a^4x_0+\frac{a^2}{3u}\right)[\ln(ua^2R_0^2)+C_{A1}]$$

$$-\frac{a^2}{3u}+\frac{4}{45}ua^6x_0^2\,{}_2F_2\left(1,1;3,\frac{7}{2};\;ua^2x_0\right)-\frac{8}{315}ua^6x_0y_0\,{}_2F_2\left(1,1;2,\frac{9}{2};\;ua^2x_0\right)$$

$$+\left(\frac{4}{15}u^2a^8x_0^2-\frac{2}{3}ua^6x_0+\frac{1}{2}a^4\right)r_0^2C_{A2}+\left(\frac{2}{7}u^2a^8x_0y_0-ua^6y_0\right)r_0^2C_{A3}\quad\Big]$$

$$+\int_0^1 du\,exp\left[-\frac{w}{u}a^2\overline{MA}^2-\frac{1-w}{u}a^2\overline{MB}^2\right]f_0^{(2)}f_{0B}^{(2)}$$

$$\Big[\ \frac{C_{A0}}{r_0^2}+\left(\frac{4}{45}\frac{a^4}{u^2}y_0-\frac{2}{9}\frac{a^4}{u^2}x_0+\frac{a^2}{3u}\right)\left[\ln\left(\frac{a^2}{u}R_0^2\right)+C_{A1}\right]$$

$$-\frac{a^2}{3u}+\frac{4}{45}\frac{a^6}{u^3}x_0^2\,{}_2F_2\left(1,1;3,\frac{7}{2};\;ua^2x_0\right)-\frac{8}{315}\frac{a^6}{u^3}x_0y_0\,{}_2F_2\left(1,1;2,\frac{9}{2};\;ua^2x_0\right)$$

$$+\left(\frac{4}{15}\frac{a^8}{u^4}x_0^2-\frac{2}{3}\frac{a^6}{u^3}x_0+\frac{1}{2}\frac{a^4}{u^2}\right)r_0^2C_{A2}+\left(\frac{2}{7}\frac{a^8}{u^4}x_0y_0-\frac{a^6}{u^3}y_0\right)r_0^2C_{A3}\quad\Big]\ \Big\}$$

$$+O(R_0^4)\qquad(3.2.48)$$

where $f_0^{(1)}$ is given by Eq. (3.1.45), $f_0^{(2)}$ is given by (3.1.52), x_0 is given by (3.1.59), y_0 is given by (3.1.60), C_{A0} is given by (3.2.35), C_{A1} is given by (3.2.36), C_{A2} is given by (3.2.37), C_{A3} is given by (3.2.45), and $f_{0B}^{(1)}$ and $f_{0B}^{(2)}$ are given by

$$f_{0B}^{(1)}=\left[\frac{\zeta_B^2}{2(1-w)ua^2}\int_0^1 dt_2\frac{(1-t_2)^{\varepsilon B}}{t_2^{4+\varepsilon B}}-\int_0^1 dt_2\frac{(1-t_2)^{\varepsilon B}}{t_2^{2+\varepsilon B}}\right]exp\left[-\frac{\zeta_B^2}{4(1-w)ua^2t_2^2}\right]\qquad(3.2.49)$$

and

$$f_{0B}^{(2)}=\left[\frac{u\zeta_B^2}{2(1-w)a^2}\int_0^1 dt_2\frac{(1-t_2)^{\varepsilon B}}{t_2^{4+\varepsilon B}}-\int_0^1 dt_2\frac{(1-t_2)^{\varepsilon B}}{t_2^{2+\varepsilon B}}\right]exp\left[-\frac{u\zeta_B^2}{4(1-w)a^2t_2^2}\right]\qquad(3.2.50)$$

For I_{yy}, we have it by replacing y_0 by $-\frac{1}{2}(y_0+\sqrt{3}y_2)$ in I_{zz}, Eq. (3.2.48), where y_m is given by

$$y_m=w^2S_{2m}(\overrightarrow{MA})+(1-w)^2S_{2m}(\overrightarrow{MB})+w(1-w)S_{2m}(\overrightarrow{MA},\overrightarrow{MB};1)\qquad(3.2.51)$$

in which $S_{2m}(\overrightarrow{MA},\overrightarrow{MB};1)$ is the mixed solid harmonics defined in a previous article [28] as given by

$$S_{2m}(\overrightarrow{MA},\overrightarrow{MB};1)=2MA_zMB_z-(MA_xMB_x+MA_yMB_y)\qquad(3.2.52)$$

For I_{xx}, we have it by replacing y_0 by $-\frac{1}{2}(y_0-\sqrt{3}y_2)$ in I_{zz}, Eq. (3.2.48). For I_{xy}, a similar derivation to that for I_{zz}, we have the final formula given by

$$I_{xy}=\frac{\zeta_A^{1+\varepsilon_A}\zeta_B^{1+\varepsilon_B}}{\Gamma(1+\varepsilon_A)\Gamma(1+\varepsilon_B)}\int_0^1 dw\,[w(1-w)]^{-3/2}$$

$$a^2[wMA_x+(1-w)MB_x][wMA_y+(1-w)MB_y]$$

$$\Big\{\ \int_0^1 du\,exp[-wua^2\overline{MA}^2-(1-w)ua^2\overline{MB}^2]f_0^{(1)}f_{0B}^{(1)}$$

$$\Big[\ \frac{2}{15}\ln(ua^2R_0^2)+\frac{2}{15}C_{A1}-\frac{4}{105}ua^2x_0\,{}_2F_2\left(1,1;2,\frac{9}{2};\;ua^2x_0\right)$$

$$+\left(\frac{2}{7}u^2a^4x_0-ua^2\right)r_0^2C_{A3}\quad\Big]$$

$$+\int_0^1 du\,exp\left[-\frac{w}{u}a^2\overline{MA}^2-\frac{1-w}{u}a^2\overline{MB}^2\right]f_0^{(2)}f_{0B}^{(2)}$$

$$\Big[\ \frac{2}{15u^2}\ln\left(\frac{a^2}{u}R_0^2\right)+\frac{2}{15u^2}C_{A1}-\frac{4}{105}\frac{a^2}{u^3}x_0\,{}_2F_2\left(1,1;2,\frac{9}{2};\;\frac{a^2}{u}x_0\right)$$

$$\left(\frac{2}{7}\frac{a^4}{u^4}x_0-\frac{a^2}{u^3}\right)r_0^2C_{A3}\quad\Big]\ \Big\}+O(R_0^4)\qquad(3.2.53)$$

The I_{yz} can be written as replacing $[wMA_x+(1-w)MB_x]$ by $[wMA_z+(1-w)MB_z]$ in I_{xy}, Eq. (3.2.53). The I_{zx} can be done as replacing $[wMA_y+(1-w)MB_y]$ by $[wMA_z+(1-w)MB_z]$ in I_{xy}. Of course, $I_{\eta\xi}=I_{\xi\eta}$.

The calculation of ${}_2F_2$ in Eq. (3.2.48) can be described in Appendix B.

Using the 256-point GLQ, we have the value of I_{zz}, I_{yy}, I_{xx}, and I_{zx} with 7 significant-figure precision and I_{xy} and I_{yz} with 5 significant-figure precision. We obtain $-\frac{e^4}{c^4}I_{zz} = -0.9808368(-1)$, $-\frac{e^4}{c^4}I_{yy} = -0.9808368(-1)$, $-\frac{e^4}{c^4}I_{xx} = -0.9808368(-1)$, $-\frac{e^4}{c^4}I_{xy} = -0.32330(-12)$, $-\frac{e^4}{c^4}I_{yz} = 0.22861(-12)$, and $-\frac{e^4}{c^4}I_{zx} = -0.1101417(-9)$ for the case of three hydrogen atoms located at $\vec{M} = (0,0,0)$, $\vec{A} = (-\frac{\sqrt{8}}{3}, -\sqrt{\frac{8}{3}}, \frac{2}{3})$, and $\vec{B} = (-\frac{\sqrt{8}}{3}, \sqrt{\frac{8}{3}}, \frac{2}{3})$.

Note that each main term of I_{zz}, I_{yy}, and I_{xx} is C_{A0}/r_0^2, which is very large. As the results, each value of I_{yy} and I_{xx} is the same as that of I_{zz}. Also note that each of I_{xy}, I_{yz}, and I_{zx} has not that main term. As the results, each value of I_{xy}, I_{yz}, and I_{zx} is very small comparing with that of I_{zz}.

3.3 The Term $\vec{p}\cdot V\vec{A} + \vec{A}\cdot V\vec{p}$

We evaluate the molecular integral-formula over Dirac wave functions for the term $\vec{p}\cdot V\vec{A} + \vec{A}\cdot V\vec{p}$ with potentials of the finite nucleus for the GCDD model as follows: We can easily derive the following relation:

$$\vec{p}\cdot V\vec{A} = \vec{A}\cdot V\vec{p} \tag{3.3.1}$$

Thus, we have

$$< \chi_{\mu A}|\vec{p}\cdot V\vec{A} + \vec{A}\cdot V\vec{p}|\chi_{\nu B} > = 2 < \chi_{\mu A}|\vec{A}\cdot V\vec{p}|\chi_{\nu B} > = \frac{iZ_M^2 e^3\hbar}{c^2}\sum_{\xi}\mu_{M\xi}I_{\xi} \tag{3.3.2}$$

$$\xi \in (x, y, z)$$

where

$$I_{\xi} = \frac{16}{\pi r_0^4}\int d\vec{r_M}\left(\vec{BM}\times\vec{r_M}\right)_{\xi}F_0F_1r_A^{-\varepsilon_A}\left(\frac{\varepsilon_B}{r_B^{2+\varepsilon_B}} + \frac{\zeta_B}{r_B^{1+\varepsilon_B}}\right)\exp(-\zeta_A r_A - \zeta_B r_B) \tag{3.3.3}$$

First, we evaluate I_Z as given by

$$I_z = \frac{16}{\pi r_0^4}\int d\vec{r_M}\left(\vec{BM}\times\vec{r_M}\right)_{z}F_0F_1r_A^{-\varepsilon_A}\left(\frac{\varepsilon_B}{r_B^{2+\varepsilon_B}} + \frac{\zeta_B}{r_B^{1+\varepsilon_B}}\right)\exp(-\zeta_A r_A - \zeta_B r_B) \tag{3.3.4}$$

We use Eq. (3.2.4) and the relation derived in a previous article [20] given by

$$\left(\frac{\varepsilon_B}{r_B^{2+\varepsilon_B}} + \frac{\zeta_B}{r_B^{1+\varepsilon_B}}\right)\exp(-\zeta_B r_B) = \frac{\zeta_B^{3+\varepsilon_B}}{2\sqrt{\pi}\Gamma(2+\varepsilon_B)}\int_0^\infty dS_2 S_2^{-3/2}\exp(-S_2 r_B^2)f_2 \tag{3.3.5}$$

where f_2 is given by (3.1.6). We use the Gaussian product rule, Eq. (3.1.11), the Sack's formula, Eq. (3.1.12), and Eq. (3.1.14). Then, we have

$$I_z = \frac{\zeta_A^{1+\varepsilon_A}\zeta_B^{3+\varepsilon_B}}{\Gamma(1+\varepsilon_A)\Gamma(2+\varepsilon_B)}\int_0^\infty dS_1\int_0^\infty dS_2\,(S_1S_2)^{-3/2}\exp[-S_1\overline{MA}^2 - S_2\overline{MB}^2]f_0f_2I_1^z \tag{3.3.6}$$

where f_0 is given by Eq. (3.1.4) and

$$I_1^z = \frac{16}{\pi r_0^4}\int_0^\infty dr_M\, r_M^2F_0F_1\exp[-S_{12}r_M^2]\sum_{l=0} i_l(2S_{12}\overline{MP}\,r_M)$$
$$\int d\widehat{r_M}\sum_{m=-l}^{l} Y_l^m(\widehat{MP})Y_l^m(\widehat{r_M})^*\left(\vec{BM}\times\vec{r_M}\right)_z \tag{3.3.7}$$

The angular part can be evaluated as in a previous article [24] as given by

$$\int d\widehat{r_M}\sum_{m=-l}^{l} Y_l^m(\widehat{MP})Y_l^m(\widehat{r_M})^*\left(\vec{BM}\times\vec{r_M}\right)_z$$
$$= r_M\delta_{l1}\frac{S_1}{S_{12}}\frac{\left(\vec{BM}\times\vec{MA}\right)_z}{\overline{MP}} = r_M\delta_{l1}\frac{S_1}{S_{12}}\frac{\left(\vec{MA}\times\vec{MB}\right)_z}{\overline{MP}} \tag{3.3.8}$$

Then we have

$$I_1^z = \frac{16}{\pi r_0^4}\frac{S_1}{S_{12}}\frac{\left(\vec{MA}\times\vec{MB}\right)_z}{\overline{MP}}\int_0^\infty dr_M\, r_M^3F_0F_1\exp[-S_{12}r_M^2]i_1(2S_{12}\overline{MP}r_M)$$
$$= I_1^{zin} + I_1^{zout} \tag{3.3.9}$$

where

$$I_1^{zout} = \frac{16}{\pi r_0^4}\frac{S_1}{S_{12}}\frac{\left(\vec{MA}\times\vec{MB}\right)_z}{\overline{MP}}\int_{R_0}^\infty dr_M\, r_M^3F_0F_1\exp[-S_{12}r_M^2]i_1(2S_{12}\overline{MP}r_M) \tag{3.3.10}$$

and

$$I_1^{zout} = \frac{16}{\pi r_0^4}\frac{S_1}{S_{12}}\frac{\left(\vec{MA}\times\vec{MB}\right)_z}{\overline{MP}}\int_{R_0}^\infty dr_M\, r_M^3F_0F_1\exp[-S_{12}r_M^2]i_1(2S_{12}\overline{MP}r_M) \tag{3.3.11}$$

First, we evaluate I_1^{zin}. We use the power series for the molecular incomplete gamma function, Eq. (3.1.21), and have

$$I_1^{zin} = \frac{16}{3\pi r_0^4}\frac{S_1}{S_{12}}\frac{\left(\vec{MA}\times\vec{MB}\right)_z}{\overline{MP}}\sum_{n_1,n_2=0}\frac{(-1/r_0^2)^{n_{12}}(3/2)_{n_1}(1/2)_{n_2}}{n_1!n_2!(5/2)_{n_1}(3/2)_{n_2}}$$
$$\int_0^{R_0} dr_M\, r_M^{2n_{12}+3}\exp[-S_{12}r_M^2]i_1(2S_{12}\overline{MP}r_M)$$
$$= \frac{16}{3\pi r_0^4}\frac{\left(\vec{MA}\times\vec{MB}\right)_z}{\overline{MP}}\frac{2S_1\overline{MP}}{3}\sum_{n_1,n_2=0}\frac{(-1/r_0^2)^{n_{12}}(3/2)_{n_1}(1/2)_{n_2}}{n_1!n_2!(5/2)_{n_1}(3/2)_{n_2}}$$
$$\sum_{j=0}\frac{(S_{12}^2\overline{MP}^2)^j}{j!(5/2)_j}I_{1a}^{zin} \tag{3.3.12}$$

where we use Eq. (3.1.13) and

$$I_{1a}^{zin} = \int_0^{R_0} dr_M\, r_M^{2j+2n_{12}+4}\exp[-S_{12}r_M^2] = \frac{1}{2}\int_0^{R_0^2} dx\, x^{j+n_{12}+3/2}\exp(-S_{12}x)$$
$$= \frac{1}{2}\left(\frac{1}{S_{12}}\right)^{j+n_{12}+5/2}\gamma\left(j+n_{12}+\frac{3}{2};\, S_{12}R_0^2\right)$$
$$= \frac{1}{2}\left(\frac{1}{S_{12}}\right)^{j+n_{12}+5/2}(S_{12}R_0^2)^{j+n_{12}+5/2}\frac{\Gamma(j+n_{12}+5/2)}{\Gamma(j+n_{12}+7/2)}$$

$${}_1F_1\left(j+n_{12}+\frac{5}{2}; j+n_{12}+\frac{7}{2}; -S_{12}R_0^2\right)$$

$$=\frac{1}{2}(R_0^2)^{j+n_{12}+5/2}\frac{\Gamma(j+n_{12}+5/2)}{\Gamma(j+n_{12}+7/2)}\,{}_1F_1\left(j+n_{12}+\frac{5}{2}; j+n_{12}+\frac{7}{2}; -S_{12}R_0^2\right)$$

(3.3.13)

where we use Eq. (3.1.25). Substituting Eq. (3.3.13) into (3.3.12), we have

$$I_1^{zin}=\frac{16b^5r_0}{9\pi}S_1(\overrightarrow{MA}\times\overrightarrow{MB})_z\sum_{n_1,n_2=0}\frac{(-b^2)^{n_{12}}(3/2)_{n_1}(1/2)_{n_2}}{n_1!\,n_2!\,(5/2)_{n_1}(3/2)_{n_2}}$$

$$\sum_{j=0}\frac{(S_{12}^2\overline{MP}^2R_0^2)^j}{j!\,(5/2)_j}\frac{\Gamma(j+n_{12}+5/2)}{\Gamma(j+n_{12}+7/2)}\,{}_1F_1\left(j+n_{12}+\frac{5}{2}; j+n_{12}+\frac{7}{2}; -S_{12}R_0^2\right)$$

$$=\frac{16b^5r_0}{9\pi}S_1(\overrightarrow{MA}\times\overrightarrow{MB})_z\left\{\quad S_{B1}+\left[\frac{2}{5}S_{12}^2\overline{MP}^2-S_{12}\right]R_0^2S_{B2}+O(R_0^4)\quad\right\}$$

(3.3.14)

where

$$S_{B1}=\sum_{n_1,n_2=0}\frac{(-b^2)^{n_{12}}(3/2)_{n_1}(1/2)_{n_2}}{n_1!n_2!(5/2)_{n_1}(3/2)_{n_2}}\frac{\Gamma(n_{12}+5/2)}{\Gamma(n_{12}+7/2)}\quad(3.3.15)$$

and

$$S_{B2}=\sum_{n_1,n_2=0}\frac{(-b^2)^{n_{12}}(3/2)_{n_1}(1/2)_{n_2}}{n_1!n_2!(5/2)_{n_1}(3/2)_{n_2}}\frac{\Gamma(n_{12}+7/2)}{\Gamma(n_{12}+9/2)}\quad(3.3.16)$$

Using a similar derivation to that in Appendix A for these summations, we have

(3.3.17)

$$S_{B1}=\frac{3\pi}{4b^4}-\frac{9\sqrt{2\pi}}{8b^5}$$

and

(3.3.18)

$$S_{B2}=\frac{\pi}{4b^3}-\frac{25\sqrt{\pi}}{16\sqrt{2}b^7}$$

Thus, we have

$$I_1^{zin}=S_1(\overrightarrow{MA}\times\overrightarrow{MB})_z\left\{\frac{4}{3}R_0-\sqrt{\frac{2}{\pi}}r_0+\left[\frac{2}{5}S_{12}^2\overline{MP}^2-S_{12}\right]\left(\frac{4}{9}R_0^3-\frac{25r_0^3}{9\sqrt{2\pi}}\right)\right\}+O(R_0^5)$$

(3.3.19)

Next, we evaluate I_1^{zout}. For the outer part of the finite nucleus, we use the asymptotic expansion, Eq. (3.1.22), and have

$$I_1^{zout}=2\frac{S_1}{S_{12}}\frac{(\overrightarrow{MA}\times\overrightarrow{MB})_z}{\overline{MP}}\int_{R_0}^{\infty}dr_M\frac{1}{r_M}\exp[-S_{12}r_M^2]i_1(2S_{12}\overline{MP}r_M)$$

$$=2\frac{(\overrightarrow{MA}\times\overrightarrow{MB})_z}{\overline{MP}}\frac{2S_1\overline{MP}}{3}\sum_{j=0}\frac{(S_{12}^2\overline{MP}^2)^j}{j!(5/2)_j}I_{1a}^{zout}\qquad(3.3.20)$$

where

$$I_{1a}^{zout}=\int_{R_0}^{\infty}dr_M r_M^{2j}\exp(-S_{12}r_M^2)=\frac{1}{2}\int_{R_0^2}^{\infty}dx\,x^{j-1/2}\exp(-S_{12}x)$$

$$=\frac{1}{2}\left(\frac{1}{S_{12}}\right)^{j+1/2}\Gamma\left(j+\frac{1}{2}; S_{12}R_0^2\right)\qquad(3.3.21)$$

It is easy to derive the following relation:

$$\Gamma\left(j+\tfrac{1}{2}; S_{12}R_0^2\right)=\Gamma\left(j+\tfrac{1}{2}\right)-\frac{(S_{12}R_0^2)^{j+1/2}}{j+1/2}+\frac{(S_{12}R_0^2)^{j+3/2}}{j+3/2}+O(R_0^5)\quad(3.3.22)$$

Substituting Eq. (3.3.22) into (3.3.21) and doing the resulting equation into (3.3.20), we have

$$I_1^{zout}=S_1(\overrightarrow{MA}\times\overrightarrow{MB})_z$$

$$\left\{\frac{2}{3}\frac{\sqrt{\pi}}{\sqrt{S_{12}}}\,{}_1F_1\left(\tfrac{1}{2};\tfrac{5}{2};S_{12}\overline{MP}^2\right)-\frac{4}{3}R_0-\left[\frac{2}{5}S_{12}^2\overline{MP}^2-S_{12}\right]\frac{4}{9}R_0^3\right\}+O(R_0^5)\quad(3.3.23)$$

Substituting Eq. (3.3.19) and (3.3.23) into (3.3.9) and doing the resulting equation into (3.3.5), we have

$$I_z=\frac{\zeta_A^{1+\varepsilon_A}\zeta_B^{3+\varepsilon_B}}{\Gamma(1+\varepsilon_A)\Gamma(2+\varepsilon_B)}\int_0^{\infty}dS_1\int_0^{\infty}dS_2\,(S_1S_2)^{-3/2}\exp[-S_1\overline{MA}^2-S_2\overline{MB}^2]f_0f_2$$

$$S_1(\overrightarrow{MA}\times\overrightarrow{MB})_z$$

$$\left\{\frac{2}{3}\frac{\sqrt{\pi}}{\sqrt{S_{12}}}\,{}_1F_1\left(\tfrac{1}{2};\tfrac{5}{2};S_{12}\overline{MP}^2\right)-\frac{\sqrt{2}}{\sqrt{\pi}}r_0-\left[\frac{2}{5}S_{12}^2\overline{MP}^2-S_{12}\right]\frac{25r_0^3}{9\sqrt{2\pi}}\right\}+O(R_0^5)\quad(3.3.24)$$

We evaluate the remaining integrals by the numerical integration. To do this, we first change integral variables as follows: We set $S_{12}=z$ and $\frac{S_1}{S_{12}}=w$. The Jacobian is given by Eq. (3.1.41). Further, we separate integral over z as is same as for Eq. (3.1.43). Then, we have the final formula given by

$$I_z=(\overrightarrow{MA}\times\overrightarrow{MB})_z\frac{\zeta_A^{1+\varepsilon_A}\zeta_B^{3+\varepsilon_B}}{\Gamma(1+\varepsilon_A)\Gamma(2+\varepsilon_B)}\int_0^1 dw\,w^{-1/2}(1-w)^{-3/2}$$

$$\left\{\int_0^1 du\exp[-wua^2\overline{MA}^2-(1-w)ua^2\overline{MB}^2]f_0^{(1)}f_2^{(1)}\right.$$

$$\left[\frac{2}{3}\frac{\sqrt{\pi}}{au^{3/2}}\,{}_1F_1\left(\frac{1}{2};\frac{5}{2};ua^2x_0\right)-\frac{\sqrt{2}r_0}{\sqrt{\pi}u}-\left[\frac{2}{5}ua^2x_0-1\right]\frac{25a^2r_0^3}{9\sqrt{2\pi}}\right]$$

$$+\int_0^1 du\exp[-\frac{w}{u}a^2\overline{MA}^2-\frac{1-w}{u}a^2\overline{MB}^2]f_0^{(2)}f_2^{(2)}$$

$$\left.\left[\frac{2}{3}\frac{\sqrt{\pi}}{au^{1/2}}\,{}_1F_1\left(\frac{1}{2};\frac{5}{2};\frac{a^2}{u}x_0\right)-\frac{\sqrt{2}}{\sqrt{\pi}}\frac{r_0}{u}-\left[\frac{2}{5}\frac{a^2}{u}x_0-1\right]\frac{25a^2r_0^3}{9\sqrt{2\pi}u^2}\right]\right\}+O(R_0^5)$$

(3.3.25)

where $f_0^{(1)}$ is given by Eq. (3.1.45), $f_2^{(1)}$ is given by (3.1.47), x_0 is given by (3.1.59), $f_0^{(2)}$ is given by (3.1.52), and $f_2^{(2)}$ is given by (3.1.54). Replacing $(\overrightarrow{MA}\times\overrightarrow{MB})_z$ by $(\overrightarrow{MA}\times\overrightarrow{MB})_y$ in Eq. (3.3.25), we have the final formula of I_y. Doing that by $(\overrightarrow{MA}\times\overrightarrow{MB})_x$ in (3.3.25), we have that of I_x. Using the 64-point GLQ, we have the value of I_z, I_y, and I_x as given by $\frac{ie^3\hbar}{c^2}I_z=-0.97838414(-5)i$, $\frac{ie^3\hbar}{c^2}I_y=0$, and $\frac{ie^3\hbar}{c^2}I_x=-0.69182206(-5)i$ for the case of three hydrogen atoms located at $\vec{M}=(0,0,0)$, $\vec{A}=(-\frac{\sqrt{8}}{3},-\sqrt{\frac{8}{3}},\frac{2}{3})$, and $\vec{B}=(-\frac{\sqrt{8}}{3},\sqrt{\frac{8}{3}},\frac{2}{3})\vec{B}=(-\frac{\sqrt{8}}{3},\sqrt{\frac{8}{3}},\frac{2}{3})$. Note that.

$$(\overrightarrow{MA}\times\overrightarrow{MB})_y=MA_zMB_x-MA_xMB_z=0$$

3.4 The Term $i\vec{\sigma}\cdot(\vec{p}\times V\vec{p})$

We evaluate the molecular integral-formula over Dirac wave functions for the term $i\vec{\sigma}\cdot(\vec{p}\times V\vec{p})$ with the GCDD model of V which is given by Eq. (1.7) as follows: It is easy to derive the following relation:

$$<\chi_{\mu A}|i\vec{\sigma}\cdot(\vec{p}\times V\vec{p})|\chi_{\nu B}>=iZ_M e^2\hbar^2\sum_\xi \sigma_\xi I_\xi^\sigma \quad \xi\in(x,y,z) \tag{3.4.1}$$

where

$$I_\xi^\sigma=\frac{4}{\sqrt{\pi}r_0^3}\int d\vec{r_M}\,F_1 r_A^{-\varepsilon_A}\exp(-\zeta_A r_A)(\vec{r_M}\times\nabla)_\xi r_B^{-\varepsilon_B}\exp(-\zeta_B r_B) \tag{3.4.2}$$

First, we evaluate I_z^σ as given by

$$I_z^\sigma=\frac{4}{\sqrt{\pi}r_0^3}\int d\vec{r_M}\,F_1 r_A^{-\varepsilon_A}\exp(-\zeta_A r_A)(\vec{r_M}\times\nabla)_z r_B^{-\varepsilon_B}\exp(-\zeta_B r_B) \tag{3.4.3}$$

We use the Gaussian-transforms for the Dirac wave function, Eq. (3.2.4), and for the derivative of it as in a previous article [20] as given by

$$\nabla r_B^{-\varepsilon_B}\exp(-\zeta_B r_B)=\frac{-\vec{r_B}\zeta_B^{3+\varepsilon_B}}{2\sqrt{\pi}\Gamma(2+\varepsilon_B)}\int_0^\infty dS_2\,S_2^{-3/2}\exp(-S_2 r_B^2)\,f_2 \tag{3.4.4}$$

where f_2 is given by Eq. (3.1.6). Then, we have

$$I_z^\sigma=\frac{\zeta_A^{1+\varepsilon_A}\zeta_B^{3+\varepsilon_B}}{4\pi\Gamma(1+\varepsilon_A)\Gamma(2+\varepsilon_B)}\int_0^\infty dS_1\int_0^\infty dS_2\,(S_1S_2)^{-3/2}f_0f_2I_{z1}^\sigma \tag{3.4.5}$$

where f_0 is given by Eq. (3.1.4) and

$$I_{z1}^\sigma=\frac{-4}{\sqrt{\pi}r_0^3}\int d\vec{r_M}\,(\vec{r_M}\times\vec{r_B})_z F_1\exp(-S_1r_A^2-S_2r_B^2) \tag{3.4.6}$$

We know that $\vec{r_M}\times\vec{r_B}=\vec{r_M}\times(\vec{r_M}+\vec{BM})=\vec{r_M}\times\vec{BM}=-\vec{r_M}\times\vec{MB}$. Then, we have

$$I_{z1}^\sigma=\frac{4}{\sqrt{\pi}r_0^3}\int d\vec{r_M}\,(\vec{r_M}\times\vec{MB})_z F_1\exp(-S_1r_A^2-S_2r_B^2) \tag{3.4.7}$$

Using the Gaussian product rule, Eq. (3.1.11), Sack's formula, (3.1.12), and (3.1.14), we have

$$I_{z1}^\sigma=4\pi\exp(-S_1\overline{MA}^2-S_2\overline{MB}^2)I_{z2}^\sigma \tag{3.4.8}$$

where

$$I_{z2}^\sigma=\frac{4}{\sqrt{\pi}r_0^3}\int d\vec{r_M}\,(\vec{r_M}\times\vec{MB})_z F_1\exp(-S_{12}r_M^2)\sum_{l=0} i_l(2S_{12}\overline{MP}r_M)$$
$$\sum_{m=-l}^{l} Y_l^m(\widehat{MP})\,Y_l^m(\widehat{r_M})^*$$
$$=\frac{4}{\sqrt{\pi}r_0^3}\int_0^\infty dr_M\,r_M^2F_1\exp(-S_{12}r_M^2)\sum_{l=0} i_l(2S_{12}\overline{MP}r_M)$$
$$\int \widehat{r_M}\sum_{m=-l}^{l} Y_l^m(\widehat{MP})\,Y_l^m(\widehat{r_M})^*(\vec{r_M}\times\vec{MB})_z \tag{3.4.9}$$

The angular part can be evaluated as in a previous article [24] as given by

$$\int \widehat{r_M}\sum_{m=-l}^{l} Y_l^m(\widehat{MP})\,Y_l^m(\widehat{r_M})^*(\vec{r_M}\times\vec{MB})_z=r_M\delta_{l1}\frac{(\vec{MP}\times\vec{MB})_z}{\overline{MP}} \tag{3.4.10}$$

We know $\vec{MP}\times\vec{MB}=\frac{S_1}{S_{12}}\vec{MA}\times\vec{MB}$. Thus, we have

$$I_{z2}^\sigma=\frac{4}{\sqrt{\pi}r_0^3}\frac{S_1}{S_{12}}\frac{(\vec{MA}\times\vec{MB})_z}{\overline{MP}}\int_0^\infty dr_M\,r_M^3F_1\exp(-S_{12}r_M^2)\,i_1(2S_{12}\overline{MP}r_M)=I_{z2}^{\sigma in}+I_{z2}^{\sigma out} \tag{3.4.11}$$

where

$$I_{z2}^{\sigma in}=\frac{4}{\sqrt{\pi}r_0^3}\frac{S_1}{S_{12}}\frac{(\vec{MA}\times\vec{MB})_z}{\overline{MP}}\int_0^{R_0} dr_M\,r_M^3F_1\exp(-S_{12}r_M^2)\,i_1(2S_{12}\overline{MP}r_M) \tag{3.4.12}$$

and

$$I_{z2}^{\sigma out}=\frac{4}{\sqrt{\pi}r_0^3}\frac{S_1}{S_{12}}\frac{(\vec{MA}\times\vec{MB})_z}{\overline{MP}}\int_{R_0}^\infty dr_M\,r_M^3F_1\exp(-S_{12}r_M^2)\,i_1(2S_{12}\overline{MP}r_M) \tag{3.4.13}$$

First, we evaluate $I_{z2}^{\sigma in}$. Using the power series of the molecular incomplete gamma function, Eq. (3.1.21), and doing Eq. (3.1.13), we have

$$I_{z2}^{\sigma in}=\frac{4}{3\sqrt{\pi}r_0^3}\frac{S_1}{S_{12}}\frac{(\vec{MA}\times\vec{MB})_z}{\overline{MP}}\frac{2S_{12}\overline{MP}}{3}\sum_{j=0}\frac{(S_{12}^2\overline{MP}^2)^j}{j!(5/2)_j}\sum_{n=0}\frac{(-1/r_0^2)^n(3/2)_n}{n!(5/2)_n}I_{z2a}^{\sigma in} \tag{3.4.14}$$

where

$$I_{z2a}^{\sigma in}=\int_0^{R_0}dr_M\,r_M^{2j+2n+4}\exp(-S_{12}r_M^2)=\frac{1}{2}\int_0^{R_0^2}dx\,x^{j+n+3/2}\exp(-S_{12}x)$$
$$=\frac{1}{2}\left(\frac{1}{S_{12}}\right)^{j+n+5/2}\gamma\left(j+n+\frac{5}{2};\,S_{12}R_0^2\right)$$
$$=\frac{1}{2}\left(\frac{1}{S_{12}}\right)^{j+n+5/2}(S_{12}R_0^2)^{j+n+5/2}\frac{\Gamma(j+n+5/2)}{\Gamma(j+n+7/2)}\,{}_1F_1\left(j+n+\frac{5}{2};j+n+\frac{7}{2};\,-S_{12}R_0^2\right) \tag{3.4.15}$$

Substituting Eq. (3.4.15) into (3.4.14), we have

$$I_{z2}^{\sigma in}=\frac{4b^5r_0^2}{9\sqrt{\pi}}S_1(\vec{MA}\times\vec{MB})_z\sum_{j=0}\frac{(S_{12}^2\overline{MP}^2R_0^2)^j}{j!(5/2)_j}\sum_{n=0}\frac{(-b^2)^n(3/2)_n}{n!(5/2)_n}$$
$$\frac{\Gamma(j+n+5/2)}{\Gamma(j+n+7/2)}\,{}_1F_1\left(j+n+\frac{5}{2};j+n+\frac{7}{2};\,-S_{12}R_0^2\right)$$
$$=\frac{4b^5r_0^2}{9\sqrt{\pi}}S_1(\vec{MA}\times\vec{MB})_z\sum_{n=0}\frac{(-b^2)^n(3/2)_n}{n!(5/2)_n}\frac{\Gamma(n+5/2)}{\Gamma(n+7/2)}+O(R_0^4)$$
$$=\frac{4b^5r_0^2}{9\sqrt{\pi}}S_1(\vec{MA}\times\vec{MB})_z\frac{\Gamma(5/2)}{\Gamma(7/2)}\,{}_1F_1\left(\frac{3}{2};\frac{7}{2};\,-b^2\right)+O(R_0^4)$$
$$=\frac{4b^5r_0^2}{9\sqrt{\pi}}S_1(\vec{MA}\times\vec{MB})_z\frac{3\sqrt{\pi}}{4b^3}\left(1-\frac{3}{2b^2}\right)+O(R_0^4) \tag{3.4.16}$$

In the above derivation, we use the asymptotic expansion of the CHF given by Eq. (3.1.28). Next, we evaluate $I_{z2}^{\sigma out}$. Using the asymptotic expansion of F_1, Eq. (3.1.22), we have

$$I_{z2}^{\sigma out}=\frac{S_1}{S_{12}}\frac{(\vec{MA}\times\vec{MB})_z}{\overline{MP}}\int_{R_0}^\infty dr_M\exp(-S_{12}r_M^2)\,i_1(2S_{12}\overline{MP}r_M) \tag{3.4.17}$$

Using the power series of i_1, Eq. (3.1.13), we have

$$I_{z2}^{\sigma out}=\frac{S_1}{S_{12}}\frac{(\vec{MA}\times\vec{MB})_z}{\overline{MP}}\frac{2S_{12}\overline{MP}}{3}\sum_{j=0}\frac{(S_{12}^2\overline{MP}^2)^j}{j!(5/2)_j}I_{z2a}^{\sigma out} \tag{3.4.18}$$

where

$$I_{z2a}^{\sigma out}=\int_{R_0}^\infty dr_M\,r_M^{2j+1}\exp(-S_{12}r_M^2)=\frac{1}{2}\int_{R_0^2}^\infty dx\,x^j\exp(-S_{12}x)$$

$$=\frac{1}{2}\left(\frac{1}{S_{12}}\right)^{j+1}\Gamma(j+1;\,S_{12}R_0^2)=\frac{1}{2}\left(\frac{1}{S_{12}}\right)^{j+1}\left[\ \Gamma(j+1)-\frac{(S_{12}R_0^2)^{j+1}}{j+1}\ \right]+O(R_0^4) \tag{3.4.19}$$

In the above derivation, we use Eq. (3.1.32). Substituting Eq. (3.4.19) into (3.4.18), we have

$$I_{z2}^{\sigma out}=\frac{1}{3}(\overrightarrow{MA}\times\overrightarrow{MB})_z\left[\ \frac{S_1}{S_{12}}\ {}_1F_1\left(1;\,\frac{5}{2};\,S_{12}\overline{MP}^2\right)-S_1R_0^2\ \right]+O(R_0^4) \tag{3.4.20}$$

Substituting Eq. (3.4.16) and (3.4.20) into (3.4.11), doing the resulting equation into (3.4.8), and doing it into (3.4.5), we have

$$I_z^{\sigma}=\frac{\zeta_A^{1+\varepsilon_A}\zeta_B^{3+\varepsilon_B}}{\Gamma(1+\varepsilon_A)\Gamma(2+\varepsilon_B)}\int_0^\infty dS_1\int_0^\infty dS_2(S_1S_2)^{-3/2}\exp(-S_1\overline{MA}^2-S_2\overline{MB}^2)f_0f_2$$
$$(\overrightarrow{MA}\times\overrightarrow{MB})_z\left[\ \frac{1}{3}\frac{S_1}{S_{12}}\ {}_1F_1\left(1;\,\frac{5}{2};\,S_{12}\overline{MP}^2\right)-\frac{1}{2}S_1r_0^2\ \right]+O(R_0^4) \tag{3.4.21}$$

We evaluate the remaining integrals by the numerical integration. To do this, we first change integral variables as follows: We set $S_{12}=z$ and $\frac{S_1}{S_{12}}=w$. The Jacobian is given by Eq. (3.1.41). Further, we separate integral over z as is same as for Eq. (3.1.43). Then, we have the final formula given by

$$I_z^{\sigma}=(\overrightarrow{MA}\times\overrightarrow{MB})_z\frac{\zeta_A^{1+\varepsilon_A}\zeta_B^{3+\varepsilon_B}}{\Gamma(1+\varepsilon_A)\Gamma(2+\varepsilon_B)}\int_0^1 dw\,w^{-1/2}(1-w)^{-3/2}$$
$$\Bigg\{\ \int_0^1 du\exp[-wua^2\overline{MA}^2-(1-w)ua^2\overline{MB}^2]f_0^{(1)}f_2^{(1)}$$
$$\left[\ \frac{1}{3u^2a^2}\ {}_1F_1\left(1;\,\frac{5}{2};ua^2x_0\right)-\frac{1}{2u}r_0^2\ \right]$$
$$+\int_0^1 du\exp[-\frac{w}{u}a^2\overline{MA}^2-\frac{1-w}{u}a^2\overline{MB}^2]f_0^{(2)}f_2^{(2)}$$
$$\left[\ \frac{1}{3a^2}\ {}_1F_1\left(1;\,\frac{5}{2};\,\frac{a^2}{u}x_0\right)-\frac{1}{2u}r_0^2\ \right]\ \Bigg\}+O(R_0^4) \tag{3.4.22}$$

where $f_0^{(1)}$ is given by Eq. (3.1.45), $f_2^{(1)}$ is given by (3.1.47), x_0 is given by (3.1.59), $f_0^{(2)}$ is given by (3.1.52), and $f_2^{(2)}$ is given by (3.1.54).

Replacing $(\overrightarrow{MA}\times\overrightarrow{MB})_z$ by $(\overrightarrow{MA}\times\overrightarrow{MB})_y$ in Eq. (3.4.22), we have the final formula of I_y^{σ}. Doing that by $(\overrightarrow{MA}\times\overrightarrow{MB})_x$ in (3.4.22), we have I_x^{σ}. Using the 512-point GLQ, we have $ie^2\hbar^2I_z^{\sigma}=-0.8745759(-1)i$, $ie^2\hbar^2I_x^{\sigma}=-0.6184186(-1)i$, and $ie^2\hbar^2I_y^{\sigma}=0$ for the case of three hydrogen atoms located at $\vec{M}=(0,0,0)$, $\vec{A}=(-\frac{\sqrt{8}}{3},-\sqrt{\frac{8}{3}},\frac{2}{3})$, and $\vec{B}=(-\frac{\sqrt{8}}{3},\sqrt{\frac{8}{3}},\frac{2}{3})$. Note that $(\overrightarrow{MA}\times\overrightarrow{MB})_y=MA_zMB_x-MA_xMB_z=0$.

4. Conclusion

New Gaussian-transform formulas have been derived for special derivatives of the Dirac wave function. Using these, among all necessary molecular integral-formulas for solving the molecular matrix Dirac equation (MMDE), most formulas have been derived together with those in previous articles [19-21]. All integral-formulas have been derived for the first time. We should add the Dirac wave function to our basis set for solving the MMDE.

Necessary integral-formulas to solve the MMDE are still remaining. Such are those for two-electron operators as given by

$$<\chi_\mu\chi_\kappa\left|\vec{\sigma}\cdot(\vec{p}+\vec{A})\frac{e^2}{r_{12}}\vec{\sigma}\cdot(\vec{p}+\vec{A})\right|\chi_\nu\chi_\lambda> \tag{4.1}$$

Such project is in progress.

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Appendix A. Calculation of Summations Appearing in Eq. (3.2.22)

We calculate summations in Eq. (3.2.22) as follows: We first calculate the summation given by

$$S_{A0} = \sum_{n_1 n_2 n_3=0} \frac{(-b^2)^{n_{123}} (3/2)_{n_1} (3/2)_{n_2} (1/2)_{n_3}}{n_1!\, n_2!\, n_3!\, (5/2)_{n_1} (5/2)_{n_2} (3/2)_{n_3}} \frac{\Gamma(n_{123}+5/2)}{\Gamma(n_{123}+7/2)}$$

$$= \sum_{n_1 n_2=0} \frac{(-b^2)^{n_{12}} (3/2)_{n_1} (3/2)_{n_2}}{n_1! n_2! (5/2)_{n_1} (5/2)_{n_2}} \frac{\Gamma(n_{12}+5/2)}{\Gamma(n_{12}+7/2)}\, {}_2F_2\left(n_{12}+\frac{5}{2}, \frac{1}{2};\, n_{12}+\frac{7}{2}, \frac{3}{2};\, -b^2\right) \tag{a.1}$$

where $n_{12} = n_1 + n_2$. It is easy to derive the recurrence relation:

$${}_2F_2(a_1, a_2;\, a_1+1, a_2+1; x)$$

$$= \frac{a_1}{a_1-a_2}\, {}_1F_1(a_2;\, a_2+1; x) - \frac{a_2}{a_1-a_2}\, {}_1F_1(a_1;\, a_1+1; x) \tag{a.2}$$

Using Eq. (a.2), we have

$${}_2F_2\left(n_{12}+\frac{5}{2}, \frac{1}{2};\, n_{12}+\frac{7}{2}, \frac{3}{2};\, -b^2\right)$$

$$= \frac{n_{12}+5/2}{n_{12}+2}\, {}_1F_1\left(\frac{1}{2};\, \frac{3}{2};\, -b^2\right) - \frac{1/2}{n_{12}+2}\, {}_1F_1\left(n_{12}+\frac{5}{2};\, n_{12}+\frac{7}{2};\, -b^2\right) \tag{a.3}$$

We know the asymptotic expansion of CHF from the formula number 13.5.1 in the Abramowitz and Stegun [27] as given by

$${}_1F_1\left(\frac{1}{2};\, \frac{3}{2};\, -b^2\right) = \frac{\sqrt{\pi}}{2b} \tag{a.4}$$

We know the integral representation of CHF from the formula number 13.2.1 in the Abramowitz and Stegun [27] as given by

$${}_1F_1\left(n_{12}+\frac{5}{2};\, n_{12}+\frac{7}{2};\, -b^2\right) = \frac{\Gamma(n_{12}+7/2)}{\Gamma(n_{12}+5/2)} \int_0^1 dt\, t^{n_{12}+3/2} \exp(-b^2 t) \tag{a.5}$$

Substituting Eq. (a.3) and (a.4) into (a.2) and doing the resulting equation into (a.1), we have

$$S_{A0} = \frac{\sqrt{\pi}}{2b} \sum_{n_1 n_2=0} \frac{(-b^2)^{n_{12}} (3/2)_{n_1} (3/2)_{n_2}}{n_1!\, n_2!\, (5/2)_{n_1} (5/2)_{n_2}} \frac{\Gamma(n_{12}+2)}{\Gamma(n_{12}+3)}$$

$$-\frac{1}{2} \sum_{n_1 n_2=0} \frac{(-b^2)^{n_{12}} (3/2)_{n_1} (3/2)_{n_2}}{n_1!\, n_2!\, (5/2)_{n_1} (5/2)_{n_2}} \frac{\Gamma(n_{12}+2)}{\Gamma(n_{12}+3)} \int_0^1 dt\, t^{n_{12}+3/2} \exp(-b^2 t)$$

$$= \frac{\sqrt{\pi}}{2b} \sum_{n_1=0} \frac{(-b^2)^{n_1} (3/2)_{n_1}}{n_1!\, (5/2)_{n_1}} \frac{\Gamma(n_1+2)}{\Gamma(n_1+3)}\, {}_2F_2\left(n_1+2, \frac{3}{2};\, n_1+3, \frac{5}{2};\, -b^2\right)$$

$$-\frac{1}{2} \int_0^1 dt\, t^{3/2} \exp(-b^2 t)$$

$$\sum_{n_1=0} \frac{(-b^2 t)^{n_1} (3/2)_{n_1}}{n_1! (5/2)_{n_1}} \frac{\Gamma(n_1+2)}{\Gamma(n_1+3)}\, {}_2F_2\left(n_1+2, \frac{3}{2};\, n_1+3, \frac{5}{2};\, -b^2 t\right) \tag{a.6}$$

Using Eq. (a.2), we have

$${}_2F_2\left(n_1+2, \frac{3}{2};\, n_1+3, \frac{5}{2};\, -b^2\right)$$

$$= \frac{n_1+2}{n_1+1/2}\, {}_1F_1\left(\frac{3}{2};\, \frac{5}{2};\, -b^2\right) - \frac{3/2}{n_1+1/2}\, {}_1F_1(n_1+2;\, n_1+3;\, -b^2)$$

$$= \frac{\Gamma(n_1+1/2)}{\Gamma(n_1+3/2)} \frac{\Gamma(n_1+3)}{\Gamma(n_1+2)} \frac{3\sqrt{\pi}}{4b^3} - \frac{3}{2} \frac{\Gamma(n_1+1/2)}{\Gamma(n_1+3/2)} \frac{\Gamma(n_1+3)}{\Gamma(n_1+2)} \int_0^1 ds\, s^{n_1+1} \exp(-b^2 s) \tag{a.7}$$

and

$${}_2F_2\left(n_1+2, \frac{3}{2};\, n_1+3, \frac{5}{2};\, -b^2 t\right)$$

$$= \frac{n_1+2}{n_1+1/2}\, {}_1F_1\left(\frac{3}{2};\, \frac{5}{2};\, -b^2 t\right) - \frac{3/2}{n_1+1/2}\, {}_1F_1(n_1+2;\, n_1+3;\, -b^2 t)$$

$$= \frac{\Gamma(n_1+1/2)}{\Gamma(n_1+3/2)} \frac{\Gamma(n_1+3)}{\Gamma(n_1+2)} \frac{\Gamma(5/2)}{\Gamma(3/2)} \int_0^1 ds\, \sqrt{s} \exp(-b^2 ts)$$

$$- \frac{3}{2} \frac{\Gamma(n_1+1/2)}{\Gamma(n_1+3/2)} \frac{\Gamma(n_1+3)}{\Gamma(n_1+2)} \int_0^1 ds\, s^{n_1+1} \exp(-b^2 s) \tag{a.8}$$

Substituting Eq. (a.7) and (a.8) into (a.6), we have

$$S_{A0} = \frac{3\pi}{8b^4} \sum_{n_1=0} \frac{(-b^2)^{n_1} (3/2)_{n_1} \Gamma(n_1+1/2)}{n_1!\, (5/2)_{n_1} \Gamma(n_1+3/2)}$$

$$-\frac{3\sqrt{\pi}}{4b} \sum_{n_1=0} \frac{(-b^2)^{n_1} (3/2)_{n_1} \Gamma(n_1+1/2)}{n_1!\, (5/2)_{n_1} \Gamma(n_1+3/2)} \int_0^1 ds\, s^{n_1+1} \exp(-b^2 s)$$

$$-\frac{1}{2} \int_0^1 dt\, t^{3/2} \exp(-b^2 t)$$

$$\left[\sum_{n_1=0} \frac{(-b^2 t)^{n_1} (3/2)_{n_1} \Gamma(n_1+1/2)}{n_1!\, (5/2)_{n_1} \Gamma(n_1+3/2)} \int_0^1 ds\, \sqrt{s} \exp(-b^2 ts) \right.$$

$$\left. -\frac{3}{2} \sum_{n_1=0} \frac{(-b^2 t)^{n_1} (3/2)_{n_1} \Gamma(n_1+1/2)}{n_1!\, (5/2)_{n_1} \Gamma(n_1+3/2)} \int_0^1 ds\, s^{n_1+1} \exp(-b^2 s) \right]$$

$$= \frac{3\pi}{8b^4} \frac{\Gamma(1/2)}{\Gamma(3/2)}\, {}_1F_1\left(\frac{1}{2};\, \frac{5}{2};\, -b^2\right)$$

$$-\frac{3\sqrt{\pi}\,\Gamma(1/2)}{4b\ \ \Gamma(3/2)} \int_0^1 ds\, s \exp(-b^2 s)\ {}_1F_1\left(\frac{1}{2};\, \frac{5}{2};\, -b^2 s\right)$$

$$-\frac{3}{4} \int_0^1 dt\, t^{3/2} \exp(-b^2 t)$$

$$\left[\int_0^1 ds\, \sqrt{s} \exp(-b^2 ts)\, \frac{\Gamma(1/2)}{\Gamma(3/2)}\, {}_1F_1\left(\frac{1}{2};\, \frac{5}{2};\, -b^2 t\right) \right.$$

$$\left. \int_0^1 ds\, s \exp(-b^2 s) \frac{\Gamma(1/2)}{\Gamma(3/2)}\, {}_1F_1\left(\frac{1}{2};\, \frac{5}{2};\, -b^2 ts\right) \right] \tag{a.9}$$

We use the asymptotic expansion of the CHF from the formula number 13.5.1 in the Abramowitz and Stegun [27] as given by

$${}_1F_1\left(\frac{1}{2};\, \frac{5}{2};\, -b^2\right) = \frac{\Gamma(5/2)}{b}\left(1 - \frac{1}{2b^2}\right) \tag{a.10}$$

We use the integral representation of the CHF from the formula number 13.2.1 in the Abramowitz and Stegun [27] as given by

$${}_1F_1\left(\frac{1}{2};\, \frac{5}{2};\, -b^2 s\right) = \frac{3}{2} \int_0^1 du\, u^{-1/2} (1-u) \exp(-b^2 su) \tag{a.11}$$

$${}_1F_1\left(\frac{1}{2};\, \frac{5}{2};\, -b^2 t\right) = \frac{3}{2} \int_0^1 du\, u^{-1/2} (1-u) \exp(-b^2 tu) \tag{a.12}$$

and

$${}_1F_1\left(\frac{1}{2};\, \frac{5}{2};\, -b^2 ts\right) = \frac{3}{2} \int_0^1 du\, u^{-1/2} (1-u) \exp(-b^2 tsu) \tag{a.13}$$

Substituting Eq. (a.10), (a.11). (a.12), and (a.13) into (a.9), we have

$$S_{A0} = \frac{9\pi^{3/2}}{16b^5}\left(1 - \frac{1}{2b^2}\right) - \frac{9\sqrt{\pi}}{8b} \int_0^1 du\, u^{-1/2} (1-u) \int_0^1 ds\, s \exp[-b^2 s(1+u)]$$

$$-\frac{9}{8}\int_0^1 ds\,\sqrt{s}\int_0^1 du\,u^{-1/2}(1-u)\int_0^1 dt\,t^{3/2}\exp[-b^2t(1+s+u)]$$

$$+\frac{9}{8}\int_0^1 ds\,s\int_0^1 du\,u^{-1/2}(1-u)\int_0^1 dt\,t^{3/2}\exp[-b^2t(1+s+su)] \quad \text{(a.14)}$$

We know the integral representation is nothing but the CHF as given by

$$\int_0^1 ds\,s\exp[-b^2s(1+u)] = \frac{\Gamma(2)}{\Gamma(3)}\,{}_1F_1(2;3;\,-b^2(1+u))$$

$$= \frac{\Gamma(2)}{\Gamma(3)}\frac{\Gamma(3)}{[b^2(1+u)]^2} \quad \text{(a.15)}$$

$$\int_0^1 dt\,t^{3/2}\exp[-b^2t(1+s+u)] = \frac{\Gamma(5/2)}{\Gamma(7/2)}\,{}_1F_1\left(\frac{5}{2};\frac{7}{2};\,-b^2(1+s+u)\right)$$

$$= \frac{\Gamma(5/2)}{\Gamma(7/2)}\frac{\Gamma(7/2)}{[b^2(1+s+u)]^{5/2}} \quad \text{(a.16)}$$

and

$$\int_0^1 dt\,t^{3/2}\exp[-b^2t(1+s+su)] = \frac{\Gamma(5/2)}{\Gamma(7/2)}\,{}_1F_1\left(\frac{5}{2};\frac{7}{2};\,-b^2(1+s+su)\right)$$

$$= \frac{\Gamma(5/2)}{\Gamma(7/2)}\frac{\Gamma(7/2)}{[b^2(1+s+su)]^{5/2}} \quad \text{(a.17)}$$

We use the asymptotic expansion of CHF in Eq. (a.15), (a.16) and (a.17). Substituting Eq. (a.15), (a.16), and (a.17) into (a.14), we have

$$S_{A0} = \frac{9\pi^{3/2}}{16b^5} - \frac{9\pi^{3/2}}{32b^7} - \frac{9\sqrt{\pi}}{8b^5}\int_0^1 du\frac{u^{-1/2}}{(1+u)^2} + \frac{9\sqrt{\pi}}{8b^5}\int_0^1 du\frac{\sqrt{u}}{(1+u)^2}$$

$$-\frac{27\sqrt{\pi}}{32b^5}\int_0^1 ds\int_0^1 du\frac{\sqrt{s}\,u^{-1/2}}{(1+s+u)^{5/2}} + \frac{27\sqrt{\pi}}{32b^5}\int_0^1 ds\int_0^1 du\frac{\sqrt{s}\sqrt{u}}{(1+s+u)^{5/2}}$$

$$+\frac{27\sqrt{\pi}}{32b^5}\int_0^1 ds\int_0^1 du\frac{s\,u^{-1/2}}{(1+s+su)^{5/2}} - \frac{27\sqrt{\pi}}{32b^5}\int_0^1 ds\int_0^1 du\frac{s\sqrt{u}}{(1+s+su)^{5/2}} \quad \text{(a.18)}$$

Each value of integrals appearing in Eq. (a.18) is a constant. Each constant value can be evaluated as follows: We use the formula number 2.213.4 and 2.211 of Gradshteyn and Ryzhik [23] given by

$$\int dx\frac{1}{(a+bx)^2\sqrt{x}} = \frac{\sqrt{x}}{a(a+bx)} + \frac{1}{2a}\int dx\frac{1}{(a+bx)\sqrt{x}} \quad \text{(a.19)}$$

and

$$\int dx\frac{1}{(a+bx)\sqrt{x}} = \frac{2}{\sqrt{ab}}arctg\sqrt{\frac{bx}{a}} \quad \text{(a.20)}$$

where $arctg\ x = arctangent\ x$. Using Eq. (a.19) and (a.20), we have

$$\int_0^1 du\frac{u^{-1/2}}{(1+u)^2} = \frac{1}{2} + \frac{\pi}{4} \quad \text{(a.21)}$$

and

$$\int_0^1 du\frac{u^{1/2}}{(1+u)^2} = -\frac{1}{2} + \frac{\pi}{4} \quad \text{(a.22)}$$

We use the formula number 2.3.8.1 of the Japanese formula book [29] as given by

$$\int_0^a dx\ x^{\alpha-1}(a-x)^{\beta-1}(x+z)^{-\rho}\exp(-px)$$

$$= B(\alpha,\beta)z^{-\rho}a^{\alpha+\beta-1}\Phi_1\left(\alpha,\rho,\alpha+\beta;\,-\frac{1}{z},-p\right)$$

$$Re(\alpha) > 0, Re(\beta) > 0, z > 0 \quad \text{(a.23)}$$

where $B(\alpha,\beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}$ is the beta function and $\Phi_1(a_1,a_2,c_1;\,x_1,x_2)$ is given by

$$\Phi_1(a_1,a_2,c_1;\,x_1,x_2) = \sum\frac{x_1^{k_1}x_2^{k_2}}{k_1!k_2!}\frac{(a_1)_{k_1+k_2}(a_2)_{k_1}}{(c_1)_{k_1+k_2}} \quad \text{(a.24)}$$

Taking the limit as $p \to 0$ in Eq. (a.23), we have

$$\int_0^a dx\frac{x^{\alpha-1}(a-x)^{\beta-1}}{(x+z)^\rho} = B(\alpha,\beta)z^{-\rho}a^{\alpha+\beta-1}\,{}_2F_1\left(\rho,\alpha;\,\alpha+\beta;\,-\frac{1}{z}\right) \quad \text{(a.25)}$$

We know the Kummer transformation as given by

$${}_2F_1(a_1,a_2;\,c_1;x) = (1-x)^{-a_1}\,{}_2F_1\left(a_1,c_1-a_2;\,c_1;\,\frac{-x}{1-x}\right) \quad \text{(a.26)}$$

Applying Eq. (a.26) to (a.25), we have

$$\int_0^a dx\frac{x^{\alpha-1}(a-x)^{\beta-1}}{(x+z)^\rho} = \frac{B(\alpha,\beta)}{(1+z)^\rho}a^{\alpha+\beta-1}\,{}_2F_1\left(\beta,\rho;\,\alpha+\beta;\,\frac{1}{1+z}\right) \quad \text{(a.27)}$$

Taking $a = 1$ and $z = \frac{a_2}{a_1}$, we have

$$\int_0^1 dx\frac{x^{\alpha-1}(1-x)^{\beta-1}}{(a_1x+a_2)^\rho} = \frac{B(\alpha,\beta)}{(a_1+a_2)^\rho}\,{}_2F_1\left(\beta,\rho;\,\alpha+\beta;\,\frac{a_1}{a_1+a_2}\right) \quad \text{(a.28)}$$

$$Re(\alpha) > 0, Re(\beta) > 0, a_1a_2 > 0$$

Applying Eq. (a.28) with $\alpha = 1/2$, $\beta = 1$, and $\rho = 5/2$ to the integral $\int_0^1 ds\int_0^1 du\frac{\sqrt{s}\,u^{-1/2}}{(1+s+u)^{5/2}}$, taking $a_1 = 1$ and $a_2 = 1+s$, and using the Kummer transformation, we have

$$\int_0^1 ds\int_0^1 du\frac{\sqrt{s}\,u^{-1/2}}{(1+s+u)^{5/2}} = 2\int_0^1 ds\frac{\sqrt{s}}{(2+s)^{3/2}(1+s)} + \frac{4}{3}\int_0^1 ds\frac{\sqrt{s}}{(2+s)^{3/2}(1+s)^2} = C_{A0a} \quad \text{(a.29)}$$

The right-hand side of Eq. (a.29) can be evaluated by the 4096-point GLQ and we have $C_{A0a} = 0.3132315213$ (which is in 10 significant-figure precision). A similar derivation to the above, we have

$$\int_0^1 ds\int_0^1 du\frac{s\,u^{-1/2}}{(1+s+su)^{5/2}} = 2\int_0^1 ds\frac{s}{(1+2s)^{3/2}(1+s)} + \frac{4}{3}\int_0^1 ds\frac{s^2}{(1+2s)^{3/2}(1+s)^2} = C_{A0b} \quad \text{(a.30)}$$

The right-hand side of Eq. (a.30) can be evaluated by the 64-point GLQ and we have $C_{A0b} = 0.2459321581$. Also, a similar derivation to the above, we have

$$\int_0^1 ds\int_0^1 du\frac{\sqrt{s}\sqrt{u}}{(1+s+u)^{5/2}} = \frac{2}{3}\int_0^1 ds\frac{\sqrt{s}}{(2+s)^{3/2}(1+s)} = C_{A0c} \quad \text{(a.31)}$$

Using the 4096-point GLQ, we have $_{0c} = 0.7166865812(-1)$. Again, a similar derivation to the above, we have

$$\int_0^1 ds\int_0^1 du\frac{s\sqrt{u}}{(1+s+su)^{5/2}} = \frac{2}{3}\int_0^1 ds\frac{s}{(1+2s)^{3/2}(1+s)} = C_{A0d} \quad \text{(a.32)}$$

Using the 64-point GLQ, we have $C_{A0d} = 0.6729936319(-1)$. Thus, we have the final formula given by

$$S_{A0} = \frac{9\pi^{3/2}}{16b^5} - \frac{9\pi^{3/2}}{32b^7} - \frac{9\sqrt{\pi}}{8b^5} - \frac{27\sqrt{\pi}}{32b^5}(C_{A0a} - C_{A0b} - C_{A0c} + C_{A0d}) \tag{a.33}$$

Next, we calculate the second summation given by

$$S_{A1} = \sum_{n_1 n_2 n_3=0} \frac{(-b^2)^{n_{123}} (3/2)_{n_1} (3/2)_{n_2} (1/2)_{n_3}}{n_1! n_2! n_3! (5/2)_{n_1} (5/2)_{n_2} (3/2)_{n_3}} \frac{\Gamma(n_{123}+7/2)}{\Gamma(n_{123}+9/2)} \tag{a.34}$$

With a similar derivation to that for S_{A0}, we have the final formula given by

$$S_{A1} = \frac{9\pi}{16b^4} C_{A1a} - \frac{9\sqrt{\pi}}{4b^7} C_{A1b} - \frac{135\sqrt{\pi}}{64b^7}(C_{A1c} - C_{A1d}) \tag{a.35}$$

where

$$C_{A1a} = \int_0^1 du \int_0^1 dv \sqrt{uv} \exp(-b^2 uv) = 0.9961218237(-2) \tag{a.36}$$

The term C_{A1a} is appearing in Eq. (3.1.26). For the term C_{A1b}, using 2048-point GLQ, we have

$$C_{A1b} = \int_0^1 du \int_0^1 dv \frac{\sqrt{uv}}{(1+uv)^3} = 0.2079827971 \tag{a.37}$$

For the term C_{A1c}, using Eq. (a.28) with $a_1 = u$, $a_2 = 1+s$, $\alpha = 3/2$, $\beta = 1$, and $\rho = 7/2$, doing the Kummer transformation, doing (a.28) again with $a_1 = 1$, $a_2 = 1+s$, $\alpha = 3/2$, $\beta = 1$, and $\rho = 7/2$ for the resulting equation, doing the Kummer transformation again, and doing the 4096-point GLQ for it, we have its constant value as given by

$$C_{A1c} = \int_0^1 du \int_0^1 dv \int_0^1 ds \frac{\sqrt{suv}}{(1+s+uv)^{7/2}}$$

$$= \frac{4}{9}\int_0^1 ds \frac{\sqrt{s}}{(2+s)^{3/2}(1+s)^2} + \frac{8}{75}\int_0^1 ds \frac{\sqrt{s}\, {}_2F_1[1,5/2;7/2;1/(2+s)]}{(2+s)^{5/2}(1+s)^2}$$

$$= 0.3742687401(-1) \tag{a.38}$$

For the term C_{A1d}, using Eq. (a.28) with $a_1 = su$, $a_2 = 1+s$, $\alpha = 3/2$, $\beta = 1$, and $\rho = 7/2$, doing the Kummer transformation, doing (a.28) again with $a_1 = s$, $a_2 = 1+s$, $\alpha = 3/2$, $\beta = 1$, and $\rho = 7/2$ for the resulting equation, doing the Kummer transformation again, and doing the 64-point GLQ for it, we have its constant value as given by

$$C_{A1d} = \int_0^1 du \int_0^1 dv \int_0^1 ds \frac{s^2\sqrt{uv}}{(1+s+suv)^{7/2}}$$

$$= \frac{4}{9}\int_0^1 ds \frac{s^2}{(1+2s)^{3/2}(1+s)^2} + \frac{8}{75}\int_0^1 ds \frac{s^3\, {}_2F_1[1,5/2;7/2;s/(1+2s)]}{(1+2s)^{5/2}(1+s)^2}$$

$$= 0.1586020540(-1) \tag{a.39}$$

Further, we calculate the third summation given by

$$S_{A2} = \sum_{n_1 n_2 n_3=0} \frac{(-b^2)^{n_{123}} (3/2)_{n_1} (3/2)_{n_2} (1/2)_{n_3}}{n_1! n_2! n_3! (5/2)_{n_1} (5/2)_{n_2} (3/2)_{n_3}} \frac{\Gamma(n_{123}+9/2)}{\Gamma(n_{123}+11/2)} \tag{a.40}$$

With a similar derivation to that for S_{A0}, we have the final formula given by

$$S_{A2} = \frac{9\pi^{3/2}}{32b^7} - \frac{27\pi^{3/2}}{64b^9} - \frac{27\sqrt{\pi}}{4b^9}(C_{A2a} - C_{A2b}) - \frac{945\sqrt{\pi}}{128b^9}(C_{A2c} - C_{A2d} - C_{A2e} + C_{A2f}) \tag{a.41}$$

where

$$C_{A2a} = \int_0^1 du \frac{\sqrt{u}}{(1+u)^4} = 2\int_0^1 dx \frac{x^2}{(1+x^2)^4} \tag{a.42}$$

and

$$C_{A2b} = \int_0^1 du \frac{u^{3/2}}{(1+u)^4} = 2\int_0^1 dx \frac{x^4}{(1+x^2)^4} \tag{a.43}$$

We take formulas from a Japanese mathematical formula book [30] given by

$$\int dx \frac{x^2}{(x^2+c)^4} = -\frac{x}{6(x^2+c)^3} + \frac{x}{24c(x^2+c)^3} + \frac{x}{16c^2(x^2+c)} + \frac{1}{16c^{5/2}}\arctan\left(\frac{x}{\sqrt{c}}\right) \quad c > 0 \tag{a.44}$$

and

$$\int dx \frac{x^4}{(x^2+c)^4} = \frac{cx}{6(x^2+c)^3} - \frac{7x}{24(x^2+c)^3} + \frac{x}{16c(x^2+c)} + \frac{1}{16c^{5/2}}\arctan\left(\frac{x}{\sqrt{c}}\right) \quad c > 0 \tag{a.45}$$

where $\arctan(x) = arctangent(x)$. Using Eq. (a.44) with $c = 1$ and integrating it for the interval $[0,1]$, we have the constant value of C_{A2a} as given by $C_{A2a} = \frac{1}{24} + \frac{\pi}{32}$. Using Eq. (a.45) with $c = 1$, we have also the constant value as given by $C_{A2b} = -\frac{1}{24} + \frac{\pi}{32}$.

For the term C_{A2c}, using Eq. (a.28) with $\alpha = \frac{3}{2}$, $\beta = 1$, $\rho = \frac{9}{2}$, $a_1 = 1$, and $a_2 = 1+s$, doing the Kummer transformation, Eq. (a.26), for the resulting equation, and doing the 4096-point GLQ for it, we have the constant value as given by

$$C_{A2c} = \int_0^1 ds \int_0^1 du \frac{\sqrt{su}}{(1+s+u)^{9/2}} = \frac{2}{3}\int_0^1 ds \frac{\sqrt{s}}{(2+s)^{7/2}(1+s)} + \frac{8}{15}\int_0^1 ds \frac{\sqrt{s}}{(2+s)^{7/2}(1+s)^2} + \frac{16}{105}\int_0^1 ds \frac{\sqrt{s}}{(2+s)^{7/2}(1+s)^3}$$

$$= 0.1994662002(-1) \tag{a.46}$$

For the term C_{A2d}, using Eq. (a.28) with $\alpha = \frac{3}{2}$, $\beta = 1$, $\rho = \frac{9}{2}$, $a_1 = 1$, and $a_2 = 1+u$, doing the Kummer transformation for the resulting equation, and doing the 128-point GLQ for it, we have the constant value as given by

$$C_{A2d} = \int_0^1 ds \int_0^1 du \frac{\sqrt{s}u^{3/2}}{(1+s+u)^{9/2}} = \frac{2}{3}\int_0^1 du \frac{u^{3/2}}{(2+u)^{7/2}(1+u)} + \frac{8}{15}\int_0^1 du \frac{u^{3/2}}{(2+u)^{7/2}(1+u)^2} + \frac{16}{105}\int_0^1 du \frac{u^{3/2}}{(2+u)^{7/2}(1+u)^3}$$

$$= 0.8519836140(-2) \tag{a.47}$$

For the term C_{A2e}, similarly to C_{A2c} and using the 64-point GLQ, we have its constant value as given by

$$C_{A2e} = \int_0^1 ds \int_0^1 du \frac{s^3\sqrt{u}}{(1+s+su)^{9/2}} = \frac{2}{3}\int_0^1 ds \frac{s^3}{(1+2s)^{7/2}(1+s)}$$
$$+\frac{8}{15}\int_0^1 ds \frac{s^4}{(1+2s)^{7/2}(1+s)^2} + \frac{16}{105}\int_0^1 ds \frac{s^5}{(1+2s)^{7/2}(1+s)^3}$$
$$= 0.5697996217(-2) \quad \text{(a.48)}$$

For the term C_{A2f}, similarly to C_{A2c} and using the 64-point GLQ, we have its constant value as given by

$$C_{A2f} = \int_0^1 ds \int_0^1 du \frac{s^3 u^{3/2}}{(1+s+su)^{9/2}}$$
$$= \frac{2}{5}\int_0^1 ds \frac{s^3}{(1+2s)^{7/2}(1+s)} + \frac{4}{35}\int_0^1 ds \frac{s^4}{(1+2s)^{7/2}(1+s)^2}$$
$$= 0.2821839924(-2) \quad \text{(a.49)}$$

Appendix B. Calculation of ${}_2F_2$ Functions

We calculate ${}_2F_2\left(1,1;2\ \frac{9}{2};x\right)$ and ${}_2F_2\left(1,1;3\ \frac{7}{2};x\right)$ here. Barnes [31] showed the asymptotic expansion formula for the function ${}_pF_p(\alpha_1,\cdots,\alpha_p;\ \rho_1,\cdots,\rho_p;x)$ as given by

$$\Pi_{r=1}^{p}\left\{\frac{\Gamma(\alpha_r)}{\Gamma(\rho_r)}\right\}\ {}_pF_p\{x\} = \exp(x)x^{\Sigma\alpha-\Sigma\rho}\left\{1+\Sigma_{r=1}^{p}\frac{M_r}{x^r}+\frac{J_R}{x^R}\right\} \quad \text{(b.1)}$$

where the J_R/x^R is the error term. However, he did not show the explicit formula for M_r, then, after a numerical experiment, we have the asymptotic expansion of the ${}_2F_2\left(1,1;2\ \frac{9}{2};x\right)$ as given by

$${}_2F_2\left(1,1;2\ \frac{9}{2};x\right) = \frac{\Gamma(2)\Gamma(9/2)}{\Gamma(1)\Gamma(1)}x^{-9/2}\exp(x)\Sigma_{n=0}^{40}\frac{(1)_n(7/2)_n}{n!x^n}$$

(for $x \geq 37$) (b.2)

For $x \leq 37$, we calculate it by the power series given by

$${}_2F_2\left(1,1;2\ \frac{9}{2};x\right) = \Sigma_{n=0}^{\infty}\frac{x^n(1)_n(1)_n}{n!(2)_n(9/2)_n} \quad \text{(b.3)}$$

After a numerical experiment, we have the asymptotic expansion of the ${}_2F_2\left(1,1;3\ \frac{7}{2};x\right)$ as given by

$${}_2F_2\left(1,1;3\ \frac{7}{2};x\right) = \frac{\Gamma(3)\Gamma(7/2)}{\Gamma(1)\Gamma(1)}x^{-9/2}\exp(x)\Sigma_{n=0}^{40}\frac{(2)_n(5/2)_n}{n!x^n}$$

(for $x \geq 38$) (b.4)

For $x \leq 38$, we calculate it by the power series given by

$${}_2F_2\left(1,1;3\ \frac{7}{2};x\right) = \Sigma_{n=0}^{\infty}\frac{x^n(1)_n(1)_n}{n!(3)_n(7/2)_n} \quad \text{(b.5)}$$