Static Dipole Polarizability for the $1s\sigma$ electronic state of the $H_2^+$ molecular ion

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Abstract. The static dipole polarizability for the $1s\sigma$ electron state of the $H_2^+$ hydrogen molecular ion is calculated within Born-Oppenheimer approximation. The variational expansion with randomly chosen exponents has been used for numerical studies. The results obtained for the dipole polarizability are accurate to the nine digits.
1. Introduction

One of sample few-body systems, a H$_2^+$ molecular ion have played vital roles in the development of molecular quantum mechanics. Moreover, this ion has been considered as a model system for the formulation of many different methods and approximations and is much easier to study theoretically than experimentally, and although its physical properties have been extensively calculated, few have been measured so far.

At present, the system has been redeemed widely not only in theoretical field but in experimental sites. New type of variational expansions based on randomly chosen exponents [1, 2] have been employed successfully by many researchers for the calculation of non-relativistic energy for the vibrational $v = 0$ and rotational $J = 0$ electronic state, even more the relativistic and radiative corrections of higher order of $m\alpha$ for 1$S\sigma(v = 0, J = 0)$ state of the H$_2^+$ molecular ion [3, 4]. Within the Born-Oppenheimer approximation, the improved relativistic corrections of $m\alpha^4$ and $m\alpha^6$ orders for the ground state ($v = 0, J = 0$) of the H$_2^+$ molecular ion have been obtained in [5, 6].

There are, in addition, many theoretical precision nonadiabatic values of the electric-dipole polarizability of the ground state ($v = 0, J = 0$) of the H$_2^+$ molecular ion. Shertzer and Greene [7] had evaluated the polarizabilities of the ground state ($v = 0, J = 0$) of the H$_2^+$ and D$_2^+$ using the finite element method. Bhatia and Drachman [8] calculated the dipole polarizability of the ground states ($v = 0, J = 0$) of the ions H$_2^+$ and D$_2^+$ using the second-order perturbation theory in Hylleraas coordinate. Taylor et al [9] obtained the electric-dipole polarizabilities of the ground state of H$_2^+$ and D$_2^+$ variationally using traditional molecular physics method in which any approximation based on the size of the electron mass relative to the nucleus mass could be avoided. Moss [10] obtained rotationally averaged polarizabilities of the H$_2^+$ (0, 0) and D$_2^+$ (0, 0) from scattering theory. Yan et al [11] had derived more accurate theoretical values of the both nonrelativistic energy and dipole polarizability of ground state ($v = 0, J = 0$) of H$_2^+$ using variational wave function in Hylleraas coordinates. Hilico et al [12] had derived the most accurate results for the ground states ($v = 0, J = 0$) of hydrogen molecular ions H$_2^+$ and D$_2^+$ using the perimetric coordinates. Korobov [13] had calculated the lowest order relativistic correction to the electric-dipole polarizability of the ground state of the H$_2^+$ molecular ion.

Bishop and co-workers [14, 15, 16] had obtained the dipole polarizabilities of the ground state ($v = 0, J = 0$) of the ions in a clamped nucleus approximation. Various approaches for obtaining the polarizability in the adiabatic approximation were considered in [17].

Static dipole polarizability of the 1$S\sigma(v = 0, J = 0)$ electronic state of the the H$_2^+$ molecular ion had been calculated theoretically many times in the Born-Oppeheimer approximation [18, 19, 20, 21, 22, 23].

Furthermore, several laser spectroscopy experiments have been proposed [24, 25, 26] for high precision measurements of the rovibrational spectrum of hydrogen molecular ions H$_2^+$ and HD$^+$. 
The precision measurement of the scalar electric-dipole polarizability for the $1S\sigma(v = 0, J = 0)$ state of the $H_2^+$ molecular ion have been performed by Jacobson at al.\cite{27, 28}.

In this work our goal is to obtain more accurate values for the static dipole polarizability for the $1S\sigma(v = 0, J = 0)$ state of $H_2^+$ than in \cite{14} in the Born-Oppenheimer approximation.

We want to show that the use of the variational expansion suggested in this work allows an analytical evaluation of the singular matrix elements required for the relativistic calculations and can provide us with very accurate data.

In future studies it can be used to obtain the lowest order relativistic correction to the mean electronic dipole polarizability of the $1S\sigma(v = 0, J = 0)$ state of $H_2^+$ in the Born-Oppenheimer approximation.

In Sect. 2, we outline the theoretical method for obtaining the static dipole polarizability for the $1S\sigma(v = 0, J = 0)$ state of $H_2^+$ in the Born-Oppenheimer approximation. In Sect. 3 we consider the variational wave function and the nonrelativistic energy for this state of the $H_2^+$. Moreover, main results of numerical calculation will be presented in Tables in this section. In Sect. 4 we compare our results with the other values obtained in the Born-Oppenheimer approximation. Then a conclusion will be discussed.

2. Theory

The Schrödinger equation for the $H_2^+$ molecular ion may be solved at various different levels of approximation. In what follows, we will consider one of them; the Born-Oppenheimer approximation which means that an electron moves in the field of the clamped nuclei.

In the clamped nucleus approximation, the electronic motion is perturbed by the electric field $\mathcal{E}$, and the mean electronic dipole polarizability $\alpha(R)$ is derived as a function of the internuclear separation $R$. In this work the factor of $(1 + \epsilon) = (2m + 2)/(2m + 1)$ (details can be found in \cite{7, 8, 9, 10, 11, 12, 13}, $m$ is a mass of nucleus) in the perturbation will not be considered. Then $\alpha(R)$ is averaged over the rovibronic state. In the sum over rovibronic states approach, the adiabatic molecular wave function is written as a product of an electronic and nuclear function. In this paper, however, we do not consider the effects due to the rovibronic state, and think over only the mean electronic polarizability $\alpha(R)$ for ground state $v = 0, J = 0$ of $H_2^+$ molecular ion.

In the Born-Oppenheimer approximation the electronic wave function $\Psi_0(r; R)$ satisfies the following Schrödinger equation

$$\left[ -\frac{\hbar^2}{2m_e} \nabla_r - \frac{Z_1}{r_1} - \frac{Z_2}{r_2} \right] \Psi_0(r; R) = E_0(R) \Psi_0(r; R).$$

where $r_1$ and $r_2$ are the distances from an electron to nuclei 1 and 2, respectively.

Interaction with external electric field is given by

$$H' = d \cdot \mathcal{E}$$
where \( \mathbf{d} \) is the dipole moment and \( \mathcal{E} \) is electric field strength.

Using the perturbation theory, it is easy to present that

\[
E = E_0 + E''\mathcal{E}^2
\]

(3)

to the second order in \( \mathcal{E} \), and \( E_0 \) is the solution of Eq. (1).

If the electric field is parallel to the nuclear axis, the polarizability is expressed by

\[
\alpha_\parallel = -2E''
\]

(4)

and if it is perpendicular to the nuclear axis, the polarizability is expressed by

\[
\alpha_\perp = -2E''
\]

(5)

The mean electronic polarizability is calculated by

\[
\alpha = \frac{1}{3}(\alpha_\parallel + 2\alpha_\perp).
\]

(6)

It can be shown [14, 29] that

\[
E'' = \mathbf{B}^\dagger \mathbf{D} \mathbf{A}
\]

(7)

where \( \mathbf{B} \) is the vector of coefficients in the expansion of the first-order wave function

\[
\Psi' = \sum_n b_n \psi'_n
\]

(8)

(\( \psi_n \) is certain basic functions), \( \mathbf{A} \) is the vector of coefficients in the expansion of the zero-order wave function

\[
\Psi_0 = \sum_n a_n \psi_n
\]

(9)

and \( \mathbf{D} \) is the matrix elements with elements

\[
D_{nm} = \langle \psi'_n | d \psi'_m \rangle.
\]

(10)

The \( \mathbf{B} \) is obtained from the set of inhomogeneous equations:

\[
(\mathbf{H} - E_0 \mathbf{S}) \mathbf{B} = -\mathbf{D} \mathbf{A}
\]

(11)

where the matrix elements of \( \mathbf{H} \) and \( \mathbf{S} \) are \( \langle \psi'_n | H_0 \psi'_m \rangle \) and \( \langle \psi'_n | \psi'_m \rangle \), respectively.

3. Variational approximation and numerical results

The variational wave function for the \( 1s\sigma (v = 0, J = 0) \) state of \( \text{H}_2^+ \) should be symmetrized and is constructed as follows

\[
\Psi_0 = \sum_{i=1}^{\infty} a_i (e^{-\alpha_i r_1 - \beta_i r_2} + e^{-\beta_i r_1 - \alpha_i r_2}).
\]

(12)

Parameters \( \alpha_i \) and \( \beta_i \) are generated in a quasi-random manner

\[
\alpha_i = \left[ \frac{1}{2} i (i + 1) \sqrt{p_\alpha} \right] (A_2 - A_1) + A_1
\]

\[
[x] \text{ designates the fractional part of } x, \ p_\alpha \text{ is a prime number, an interval } [A_1, A_2] \text{ is a real variational interval, which has to be optimized. Parameters } \beta_i \text{ are obtained in a}
\]
similar way. Details of the method and discussion of various aspects of its application can be found in [1, 2].

If the electric field is parallel to the nuclear axis, then

\[ d_z = -\frac{r_1^2 - r_2^2}{2R}, \]

and the perturbed function \( \Psi' \) have a form

\[ \Psi'_\parallel = \sum_{i=1}^{\infty} b_i (e^{-\alpha_i r_1 - \beta_i r_2} + e^{-\beta_i r_1 - \alpha_i r_2}). \] (14)

If the electric field is perpendicular to the nuclear axis, then

\[ d_x = -r \cos \phi, \]

and the perturbed function is taken the form

\[ \Psi'_\perp = r \cos \phi \sum_{i=1}^{\infty} b_i (e^{-\alpha_i r_1 - \beta_i r_2} + e^{-\beta_i r_1 - \alpha_i r_2}), \] (15)

where \( r \) is a distance from center along internuclear axis,

\[ r = \frac{1}{2R} \sqrt{2r_1^2 r_2^2 + 2r_1^2 R^2 + 2r_2^2 R^2 - r_1^4 - r_2^4 - R^4}. \]

In Table 1 we show variational parameters employed in the calculation of energy values \( E_0 \) and unperturbed wave function \( \Psi_0 \) at internuclear distance \( R = 2.0 \text{ a.u.} \). Using this type of variational parameters leads to the very fast convergence.

| Table 1. | Variational parameters and number of basic functions (\( n_i \)) for different subsets of the variational wave function with \( N = 100 \). Intervals [\( A_1, A_2 \)] and [\( B_1, B_2 \)] correspond to part of a randomly chosen parameters \( \alpha_i \) and \( \beta_i \) [see Eq. (13) for details], respectively, for the bond length \( R = 2.0 \text{ a.u.} \). Prime numbers are \( p_\alpha = 2, p_\beta = 3 \). |
|---|---|---|---|---|
| \( N \) | \( A_1 \) | \( A_2 \) | \( B_1 \) | \( B_2 \) |
| \( i=1 \) | 50 | 0.00 | 1.50 | 0.00 | 0.40 |
| \( i=2 \) | 50 | 0.20 | 2.00 | 1.00 | 6.00 |

In Table 2 we present a comparison of the wave functions for the ground state (\( v = 0, J = 0 \)) of the \( \text{H}_2^+ \) molecular ion at bond length \( R = 2.0 \text{ a.u.} \). The variationally obtained values of the \( \Psi_0 \) wave function are more accurate than the previous ones.

In Table 3, the convergence of both \( E_0(R = 2.0 \text{ a.u.}) \) and \( \Psi_0(r = 2.0 \text{ a.u.}; R = 2.0 \text{ a.u.}) \) is presented. In this calculation the variational parameters presented in Table 1 are used.

In Tables 4 the mean electronic polarizability for the \( 1s\sigma \) electronic state of \( \text{H}_2^+ \) molecular ion and comparison with [14] are presented. The estimated accuracy of obtained values is nine significant digits. In Table 5 the convergence of \( \alpha_\parallel \) and \( \alpha_\perp \)
Table 2. The wave function for the $1s\sigma_g$ electron state of the $H^+_2$ molecular ion at bond length $R = 2.0$ a.u.

| $r$ (a.u.) | $\Psi_0$ (a.u.) | $r$ (a.u.) | $\Psi_0$ (a.u.) |
|-----------|----------------|-----------|----------------|
| 0.00      | 0.315          | 0.00      | 0.206          |
| 0.10      | 0.315          | 0.10      | 0.180          |
| 0.20      | 0.319          | 0.20      | 0.157          |
| 0.30      | 0.326          | 0.30      | 0.137          |
| 0.40      | 0.335          | 0.40      | 0.120          |
| 0.50      | 0.347          | 0.50      | 0.104          |
| 0.60      | 0.362          | 0.60      | 9.128          |
| 0.70      | 0.380          | 0.70      | 7.955          |
| 0.80      | 0.402          | 0.80      | 6.931          |
| 0.90      | 0.428          | 0.90      | 6.036          |
| 1.00      | 0.458          | 1.00      | 5.256          |
| 1.10      | 0.401          | 1.10      | 4.575          |
| 1.20      | 0.352          | 1.20      | 3.981          |
| 1.30      | 0.308          | 1.30      | 3.463          |
| 1.40      | 0.270          | 1.40      | 3.012          |
| 1.50      | 0.236          | 1.50      | 7.385          |

Table 3. Convergence of both energy at bond length $R = 2.0$ a.u. and wave function at distance from center along internuclear axis $r = 2.0$ a.u. for the $1s\sigma_g$ electron state of the $H^+_2$ molecular ion.

| $N$ | $E_0$ (a.u.) | $\Psi_0$ (a.u.) |
|-----|--------------|----------------|
| 60  | -1.10263421449494645849 | 0.1200445507422 |
| 70  | -1.10263421449494646060 | 0.1200445508059 |
| 90  | -1.10263421449494646150 | 0.1200445508281 |
| 100 | -1.10263421449494646150 | 0.1200445508283 |

with the increase in the expansion length of $\Psi_{1||}$ and $\Psi_{1\perp}$ (Eqs. (14)-(15)) is demonstrated for some values of internuclear distance $R$.

Numerical evaluation of the matrix elements for operators in (1) and (5) is expounded in the Appendix.

In order to get accurate results we use three sets of basic function of the type (12) (in a spirit of (1)) for small values of internuclear distance $R$, two sets for intermediate and large values of $R$, respectively. Total number of the basic function varies from $N = 110$ to $N = 300$. In our calculations arithmetics of sextuple precision (about 48 decimal digits) implemented as a FORTRAN90 module has been used. In all tables the
Table 4. The dipole polarizability for the $1s\sigma(v = 0, J = 0)$ state of $H_2^+$

| $R$ | $\alpha\parallel$ | $\alpha\perp$ | $\alpha\parallel$ | $\alpha\perp$ | $\alpha$ |
|-----|----------------|-------------|----------------|-------------|--------|
| 0.05 | 0.284 434 63 | 0.284 064 67 | 0.284 187 99 |
| 0.10 | 0.293 065 94 | 0.291 556 44 | 0.292 059 61 |
| 0.20 | 0.323 180 58 | 0.316 745 01 | 0.318 890 20 |
| 0.30 | 0.367 729 08 | 0.352 002 47 | 0.357 244 67 |
| 0.40 | 0.425 732 10 | 0.395 076 94 | 0.405 295 33 |
| 0.50 | 0.497 558 14 | 0.444 803 03 | 0.462 888 07 |
| 0.60 | 0.584 328 47 | 0.500 513 40 | 0.528 451 76 |
| 0.70 | 0.687 676 16 | 0.561 784 00 | 0.603 748 05 |
| 0.80 | 0.809 649 71 | 0.628 314 08 | 0.688 759 29 |
| 0.90 | 0.952 682 22 | 0.699 865 38 | 0.784 137 66 |
| 1.00 | 0.111 959(1) | 0.776 229 40 | 0.890 684 27 |
| 1.10 | 0.179 816 83(1) | 0.103 221 75(1) | 0.128 753 44(1) |
| 1.20 | 0.244 196 01(1) | 0.122 321 10(1) | 0.162 946 07(1) |
| 1.30 | 0.380 894 55(1) | 0.153 548 15(1) | 0.229 330 28(1) |
| 1.40 | 0.507 764 90(1) | 0.175 764 86(1) | 0.286 431 54(1) |
| 1.50 | 0.772 496 21(1) | 0.210 563 48(1) | 0.397 874 39(1) |
| 1.60 | 0.101 494 85(2) | 0.234 342 47(1) | 0.494 544 48(1) |
| 1.70 | 0.151 541 85(2) | 0.270 144 97(1) | 0.685 236 15(1) |
| 1.80 | 0.196 995 06(2) | 0.293 660 88(1) | 0.852 424 12(1) |
| 1.90 | 0.374 330 77(2) | 0.349 066 59(1) | 1.048 048 03(2) |
| 2.00 | 0.700 473 12(2) | 0.396 437 11(1) | 0.259 920 18(2) |
| 2.10 | 0.129 572 67(3) | 0.433 014 66(1) | 0.460 776 54(2) |
| 2.20 | 0.237 462 00(3) | 0.457 943 66(1) | 0.822 069 74(2) |
| 2.30 | 0.431 696 21(3) | 0.472 234 01(1) | 0.147 046 96(3) |
| 2.40 | 0.779 110 33(3) | 0.478 162 22(1) | 0.262 891 04(3) |
| 2.50 | 0.139 675 65(4) | 0.478 432 00(1) | 0.468 775 05(3) |
| 2.60 | 0.248 888 50(4) | 0.475 481 44(1) | 0.832 798 21(3) |
| 2.70 | 0.441 080 53(4) | 0.471 132 49(1) | 0.147 340 93(4) |
| 2.80 | 0.777 895 05(4) | 0.466 548 44(1) | 0.259 609 38(4) |
| 2.90 | 0.136 601 77(5) | 0.462 359 95(1) | 0.455 647 47(4) |
| 3.00 | 0.238 968 73(5) | 0.458 835 24(1) | 0.796 864 99(4) |
| 3.10 | 0.416 635 75(5) | 0.456 027 67(1) | 0.138 908 99(5) |
| 3.20 | 0.724 216 51(5) | 0.453 880 28(1) | 0.241 435 53(5) |

factor $x$ in the brackets means $10^x$. Atomic units are used throughout.
Table 5. Convergence of dipole polarizabilities with the increase in the basic-set size of $\Psi'$

| $R$(a.u.) | $N$ | $\alpha_{\parallel}$         | $\alpha_{\perp}$         |
|----------|-----|------------------------------|----------------------------|
| 1.00     | 100 | 0.111 959 391 834 (1)        | 0.776 229 394 339          |
|          | 150 | 0.111 959 395 159 (1)        | 0.776 229 397 334          |
|          | 200 | 0.111 959 395 159 (1)        | 0.776 229 397 334          |
|          | 250 | 0.111 959 395 159 (1)        | 0.776 229 397 335          |
|          | 300 | 0.111 959 395 159 (1)        | 0.776 229 397 335          |
| 1.50     | 100 | 0.244 195 787 807 (1)        | 0.122 321 061 209 (1)      |
|          | 150 | 0.244 196 012 382 (1)        | 0.122 321 099 085 (1)      |
|          | 200 | 0.244 196 012 392 (1)        | 0.122 321 099 095 (1)      |
|          | 250 | 0.244 196 012 392 (1)        | 0.122 321 099 095 (1)      |
|          | 300 | 0.244 196 012 392 (1)        | 0.122 321 099 095 (1)      |
| 2.00     | 100 | 0.507 759 939 512 (1)        | 0.175 763 635 406 (1)      |
|          | 150 | 0.507 764 896 289 (1)        | 0.175 764 860 893 (1)      |
|          | 200 | 0.507 764 898 343 (1)        | 0.175 764 861 787 (1)      |
|          | 250 | 0.507 764 898 353 (1)        | 0.175 764 861 793 (1)      |
|          | 300 | 0.507 764 898 353 (1)        | 0.175 764 861 793 (1)      |

4. Conclusion

The mean electronic polarizability for the $1s\sigma(v = 0, J = 0)$ electron state of the $\text{H}_2^+$ hydrogen molecular ion have been accurately calculated within Born-Oppenheimer approximation. The variational expansion with randomly chosen exponents has been used for numerical studies. This type of expansion allows us to use few number of basic functions. If nonrelativistic energy values of $\text{H}_2^+(0,0)$ are required to $10^{-15}$ a.u. accuracy, then the wave functions must be accurate, at least, to this same level. The wave functions, however, are typically accurate to less than half as many significant figures as the energy. Seeing from Tables 3, the precision nonrelativistic energy value $E_0$ at bond length $R = 2.0$ a.u. can easily reach to 15-significant digits for basic function number $N = 60$ and the unperturbed wave function $\Psi_0$ have 10-significant digits using the same number of terms.

Previous calculations performed for $1S\sigma(v = 0, J = 0)$ state of $\text{H}_2^+$ molecular ion over a wide range of internuclear separations $R$ are by Dalgarno and Lewis [23], Calvert and Davison [21], Bates [20], McEachran and Smith [18], and Bishop and Cheung [14]. Both Dalgarno and Lewis [23] and Bates [20] used the oscillator strength sum rule. McEachran and Smith [18] employed the variational procedure, using the accurate two-center James [31] orbital as the perturbed function. Bishop and Cheung [14] had calculated variationally the first accurate mean electronic polarizability over a wide range of internuclear separations. Rahman [19] and Adamov et al [22] had performed
Table 6. Comparison with earlier calculations at a bond length $R = 2.0\, a.u.$

|   | $\alpha_\parallel$  | $\alpha_\perp$  |
|---|---------------------|------------------|
| 19| 5.061               | 1.758            |
| 23| 5.283               | 2.202            |
| 22| 5.173               | 1.847            |
| 21| 5.084               | 1.767            |
| 20| 5.06                | 1.76             |
| 18| 5.199               | 1.829            |
| 14| 5.077 65            | 1.757 65         |
| this work | 5.077 6490 | 1.757 6486 |

accurate first order variational calculations near the equilibrium distance $R = 2.0\, a.u.$.

In Table 6 we place the comparison of our results with the earlier ones, which demonstrate superiority of the newly obtained results. The results obtained for the dipole polarizability are accurate to the nine digits. That is two digits more accurate than in [14].

In general, the total molecular rovibronic wave function is taken a form as a product of separate electronic, vibrational and rotational wave functions, that is, $\Psi_{v,J,M} = |v(J)\rangle Y_{JM}^M(\theta, \phi)$—rovibrational wave function. Then the full static dipole polarizability can be written in the form

$$\alpha(v, J, M) = \alpha^e(v, J, M) + \alpha^\nu(v, J, M) + \alpha^r(v, J, M) \tag{16}$$

where the superscripts $e, \nu, r$ imply the electronic, vibrational and rotational parts of the static dipole polarizability, respectively, and the electronic part—$\alpha^e(v, J, M)$ can be calculated by averaging over the mean electronic polarizability (details of Eq. (16) can be found in [17]).

Seeing Eq. (16), the rovibronic effects can be taken into account by averaging over the vibrational and rotational wave functions, of quantities calculated in the Born-Oppenheimer approximation.

In the calculation of the mean electronic polarizability in this Letter the effects the electron mass respect to the nuclei mass has not been taken into account. This effects, however, must be taken into account when full three-body Hamiltonian (details can be found in [7, 9, 32]) is employed.

Using the unperturbed $\Psi_0$ and perturbed $\Psi'$ functions obtained in this paper we can calculate some expectation values of the lowest order relativistic correction (Eq. (9) in [13]) to the mean electronic polarizability $\alpha$ of the $1S\sigma$ state of $H_2^+$ molecular ion. In addition, the accurate data used in evaluation of the mean electronic polarizability $\alpha$ in this work can be employed in the calculation of relativistic correction to it. This work is in progress now.
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**Appendix: Analytical evaluation of the matrix elements**

The calculation of the matrix elements is reduced to evaluation of integrals of the type

\[
\Gamma_{lm}(\alpha, \beta) = \int r_1^{l-1} r_2^{m-1} e^{-\alpha r_1 - \beta r_2} d^3r. \tag{A-1}
\]

Integers \((l, m)\) are, in general, non-negative, but in case of singular matrix elements one of the indices can be negative.

The function \(\Gamma_{00}\) can be easily obtained

\[
\Gamma_{00}(\alpha, \beta, R) = 4\pi \frac{e^{-\beta R} - e^{-\alpha R}}{\alpha^2 - \beta^2}, \tag{A-2}
\]

where \(R\) is the distance between nuclei, then \(\Gamma_{lm}(\alpha, \beta; R)\) for non-negative \((l, m)\) may be generated from \((A-2)\) by means of relation

\[
\Gamma_{lm}(\alpha, \beta; R) = \left(-\frac{\partial}{\partial \alpha}\right)^l \left(-\frac{\partial}{\partial \beta}\right)^m \Gamma_{00}(\alpha, \beta, R). \tag{A-3}
\]

Integral \(\Gamma_{-1,0}(\alpha, \beta; R)\) is expressed by

\[
\Gamma_{-1,0}(\alpha, \beta; R) = \frac{2\pi}{R^3} \left\{ e^{\beta R} E_1(R(\alpha + \beta)) + e^{-\beta R} \ln R(\alpha + \beta) - e^{\beta R}[E_1(R(\alpha - \beta)) + \ln R(\alpha - \beta)] \right\}. \tag{A-4}
\]

Worthy to note that a function in square brackets is analytic when argument is zero. Integrals \(\Gamma_{-1,m}\) are generated from \(\Gamma_{-1,0}\) similar to \((A-3)\):

\[
\Gamma_{-1,m}(\alpha, \beta; R) = \left(-\frac{\partial}{\partial \beta}\right)^m \Gamma_{-1,0}(\alpha, \beta, R). \tag{A-5}
\]

Function \(E_1(z)\) encountered in \((A-4)\) is the exponential integral function \([33]\):

\[
E_1(z) = \Gamma(0, z) = \int_z^\infty t^{-1}e^{-t}dt.
\]

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