Relativistic corrections of order $m\alpha^6$ to the two-centre problem

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Abstract

Effective potentials of the relativistic $m\alpha^6$ order correction for the ground state of the Coulomb two-centre problem are calculated. They can be used to evaluate the relativistic contribution of that order to the energies of hydrogen molecular ions or metastable states of the antiprotonic helium atom, where precision spectroscopic data are available. In our studies we use the variational expansion based on randomly chosen exponents that permits us to achieve high numerical accuracy.

1. Introduction

In recent years several experiments on precision spectroscopy of three-body light atomic and molecular systems have become available [1–3]. That is a great challenge to theorists, since the quantum electrodynamics for the few-body bound state problem is not as well elaborated as for atoms comprised of two particles.

On the other hand, the numerical variational solution for the nonrelativistic Coulomb three-body problem has reached a very high precision. The ground state of the $\text{H}_2^+$ molecular ion has been calculated with as much as 30 digits [4] (for other examples of nonrelativistic calculations see references therein).

Accurate knowledge of both theoretical and experimental transition frequencies has the potential of improving $m_e/m_p, m_e/m_\bar{p}$, etc mass ratios [5–7]. In order to achieve this goal the important step is evaluation of the relativistic and radiative corrections for the binding energies. This can be systematically performed using series expansion of the binding energy in terms of the coupling constant, $\alpha$. The leading order relativistic and radiative corrections ($R_\infty\alpha^2, R_\infty\alpha^3$) have been obtained in [8, 9]. The main aim of this work is to calculate a contribution of order $m\alpha^6$ (or $R_\infty\alpha^4$) due to relativistic corrections for the bound electron in the nonrecoil limit. The radiative corrections to this order are known analytically [10]. A sum of these two contributions constitutes a complete $m\alpha^6$ order correction for a one-electron three-body system in a nonrecoil limit.
2. Nonrelativistic Hamiltonian and variational expansion

In what follows we consider the Coulomb two-centre problem with the nonrelativistic Hamiltonian

\[ H_0 = \frac{p^2}{2m} + V, \quad V = -\frac{Z_1}{r_1} - \frac{Z_2}{r_2}, \]

where \( r_1 \) and \( r_2 \) are the distances from an electron to nuclei 1 and 2, respectively. Atomic units, \( m_e = e = \hbar = 1 \), are used throughout.

In order to get a precise solution for the Schrödinger equation

\[ \left( \frac{p^2}{2m} + V \right) \Psi_0(r) = E_0 \Psi_0(r), \]

we use the variational approach. A variational expansion for the wavefunction of the ground state of electron is taken in the form \( Z_1 \neq Z_2 \):

\[ \Psi(r) = e^{im\varphi} r^m \sum_{i=1}^{\infty} C_i e^{-\alpha_i r_1 - \beta_i r_2}, \]

where \( r \) is the distance from an electron to the \( z \)-axis and

\[ r = \frac{1}{2R} \left( 2r_1^2 r_2^2 + 2r_1^2 R^2 + 2r_2^2 R^2 + r_1^4 - r_2^4 - R^4 \right). \]

For \( Z_1 = Z_2 \) the variational wavefunction should be symmetrized,

\[ \Psi(r_1, r_2) = e^{im\varphi} r^m \sum_{i=1}^{\infty} C_i (e^{-\alpha_i r_1 - \beta_i r_2} \pm e^{-\beta_i r_1 - \alpha_i r_2}), \]

where \((+)\) is used to get a \textit{gerade} electronic state and \((-)\) is for an \textit{ungerade} state, respectively. Parameters \( \alpha_i \) and \( \beta_i \) are generated in a quasi-random manner \([11, 12]\)

\[ \alpha_i = \left[ \frac{1}{2} i(i + 1) \sqrt{p_0} \right] (A_2 - A_1) + A_1. \]

Here \( \lfloor x \rfloor \) designates the fractional part of \( x \), \( p_0 \) is a prime number, an interval \([A_1, A_2]\) is a real variational interval, which has to be optimized. Parameters \( \beta_i \) are obtained in a similar way.

The Schrödinger equation expressed in coordinates, \( r_1, r_2, \varphi \), has a form

\[ \left\{ \frac{1}{2} \left( \frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1} \frac{\partial}{\partial r_1} \right) + \left( \frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2} \frac{\partial}{\partial r_2} \right) + \frac{r_1^2 + r_2^2 - R^2}{r_1 r_2} \frac{\partial}{\partial r_1} \frac{\partial}{\partial r_2} - \frac{m^2}{r^2} \right\} \Psi = E \Psi. \]

In order to get accurate results we use several sets of basis functions of equation (3) (or (4)) (in the spirit of [11]) with different values of variational parameters: three sets for small values of internuclear distance \( R \), and two sets for intermediate and large values of \( R \), respectively. The total number of basis functions varies from \( N = 110 \) to \( N = 250 \). Using the variational method described above the nonrelativistic energy has been obtained with accuracy of more than 20 significant digits. In these calculations arithmetic of sextuple precision (about 48 decimal digits) has been used. Earlier, in a previous paper [13] using the same variational approach the effective potentials of the Breit–Pauli Hamiltonian were calculated up to ten significant digits.

The matrix elements, which appear in this and the following sections, have been evaluated analytically; for further details see appendix A.
Relativistic corrections of order $ma^6$ to the two-centre problem

3. Breit–Pauli Hamiltonian

The leading order relativistic correction of order $ma^4$ can be expressed by the Breit–Pauli Hamiltonian:

$$H_B = -\frac{p^4}{8m^3} + \frac{1}{8m^2} \left[ Z_1 4\pi \delta(r_1) + Z_2 4\pi \delta(r_2) \right] + \left( \frac{Z_1 [r_1 \times p]}{2m^2 r_1^3} + \frac{Z_2 [r_2 \times p]}{2m^2 r_2^3} \right)s. \quad (7)$$

The spin-dependent term (the last term in equation (7)) of the Breit–Pauli Hamiltonian $H_{so}^B$ does not contribute to the energy at this order, but should be taken into account when the $ma^6$ order relativistic corrections are considered.

4. Relativistic corrections of $ma^6$ order

In this section we will assume for simplicity of notation that $H_B \equiv H_s^B$, the scalar term of $H_B$. The spin–orbit term $H_{so}^B$ will be treated separately.

Our method is based on the effective Hamiltonian approach, which is closely related to ideas of [14, 15], where a case of atomic hydrogen has been considered.

4.1. Formal expressions

The energy displacement due to the $ma^6$ order relativistic corrections can be expressed as:

$$\Delta E^{(6)} = \langle H_B Q(E_0 - H^0)^{-1} QH_B \rangle + \langle H^{(6)} \rangle. \quad (8)$$

Here $Q = I - |\psi_0\rangle \langle \psi_0|$ is a projection operator. The effective Hamiltonian corresponding to this contribution has a form [14]

$$H^{(6)} = \frac{p^6}{16m^5} + \frac{(\mathcal{E}_1 + \mathcal{E}_2)^2}{8m^3} - \frac{3\pi}{16m^2} \left[ p^2 [\rho_1 + \rho_2] + [\rho_1 + \rho_2] p^2 \right]$$

$$+ \frac{5}{128m^4} (p^4 V + V p^4) = \frac{5}{64m^4} (p^2 V p^2), \quad (9)$$

where $\mathcal{E}_i = -Z_i r_i/r_i^3$ and $\rho_i = Z_i \delta(r_i)$ ($\Delta V = 4\pi \rho$).

Separately, both contributions of (8) are divergent.

4.2. Removing divergences from the second-order contribution

The second-order perturbation term

$$\Delta E^{(2)}_B = \langle H_B Q(E_0 - H^0)^{-1} QH_B \rangle \quad (10)$$

can be evaluated by obtaining the wavefunction $\Psi_B$ as a solution of equation

$$(E_0 - H_0)\Psi_B = (H_B - \langle H_B \rangle)\Psi_0. \quad (11)$$

then the correction to the energy from equation (10) can be expressed as

$$\Delta E^{(2)}_B = \langle \Psi_0 | (H_B - \langle H_B \rangle) | \Psi_0 \rangle.$$

It is known that a formal second-order expression of the type

$$\langle \Psi_0 | \delta^3(r_1) Q(E_0 - H_0)^{-1} Q \delta^3(r_1) | \Psi_0 \rangle$$

is divergent. Similarly, $p^4 |\Psi_0\rangle$ behaves as

$$-2mp^2 V |\Psi_0\rangle \sim 8\pi m [Z_1 \delta(r_1) + Z_2 \delta(r_2)] |\Psi_0\rangle$$

at small values of $r_1, r_2$. 


In order to understand how to overcome this problem, let us consider first the atomic hydrogen \(3\)-state case. Let \(\Psi_B^{(H)}\) be a solution of equation

\[
\left[ E_0 - \left( \frac{p^2}{2m} - \frac{Z}{r} \right) \right] \Psi_B^{(H)} = Q \left[ - \frac{p^4}{8m^3} + \frac{Z\pi}{2m^2} \delta(r) \right] \Psi_B^{(H)},
\]

separating the dominant behaviour at small \(r\), the solution of above equation can be presented as

\[
\Psi_B^{(H)} = \frac{Z\Psi_0(0)}{4mr} + \tilde{\Psi}_B^{(H)},
\]

where \(\tilde{\Psi}_B^{(H)}\) is a less singular function, \(\tilde{\Psi}_B^{(H)} \sim \ln r \rightarrow 0\).

Coming back to the two-centre problem, let us try to separate the singular part of the Breit–Pauli wavefunction solution \(\Psi_B\) as follows:

\[
\Psi_B = U\Psi_0 + \tilde{\Psi}_B,
\]

where \(U = -\frac{1}{4m}V\). Substituting of equation (13) into equation (10) modifies our equations,

\[
\Delta E_B^{(2)} = \langle \Psi_0 | (H_B - \langle H_B \rangle) U | \Psi_0 \rangle + \langle \Psi_0 | (H_B - \langle H_B \rangle) | \tilde{\Psi}_B \rangle,
\]

and \(\tilde{\Psi}_B\) is a solution of

\[
(E_0 - H_0)\tilde{\Psi}_B = -(E_0 - H_0)U\Psi_0 + (H_B - \langle H_B \rangle)\Psi_0.
\]

However, the last term in equation (14a) is still divergent, the singularity from the left-hand side of this term should be eliminated as well:

\[
\langle \Psi_0 | (H_B - \langle H_B \rangle) | \tilde{\Psi}_B \rangle = \langle \Psi_0 | (H_B - \langle H_B \rangle)(E_0 - H_0)^{-1}[-(E_0 - H_0)U + (H_B - \langle H_B \rangle)] | \Psi_0 \rangle = \langle \Psi_0 | -U(E_0 - H_0)U + U(H_B - \langle H_B \rangle) | \Psi_0 \rangle + \langle \tilde{\Psi}_B | -(E_0 - H_0)U + (H_B - \langle H_B \rangle) | \Psi_0 \rangle.
\]

These transformations as can be seen are equivalent to that used by Pachucki in [16]:

\[
\begin{align*}
\{ & H_B' = H_B - (E_0 - H_0)U - U(E_0 - H_0) \\
& + (UH_B + H_BU) - 2\langle U | H_B - (E_0 - H_0)U
\}
\end{align*}
\]

The last three terms can be recast in a form of a new interaction modifying the Hamiltonian \(H^{(6)}\):

\[
H^{(6)} = (UH_B + H_BU) - 2U\langle H_B \rangle - U(E_0 - H_0)U;
\]

\[
\langle H^{(6)} \rangle = \frac{1}{32m^4} \left( p^4 V + V p^4 \right) - \frac{\pi}{4m^2} \langle V[\rho_1 + \rho_2] \rangle \]
\[
+ \frac{1}{32m^3} \langle (E_1 + E_2)^2 \rangle + \frac{1}{2m} \langle V \rangle \langle H_B \rangle.
\]

A respective transformation of the Breit–Pauli operator is

\[
H_B' = -\frac{p^4}{8m^3} + \frac{\pi}{m^2} \left[ Z_1 \delta(r_1) + Z_2 \delta(r_2) \right] - \frac{1}{4m^2} \langle E_1 + E_2 \rangle \nabla + 2U\langle H_0 - E_0 \rangle.
\]

Finally, the energy shift can be written as

\[
\Delta E^{(6)} = \langle H_B' Q(E_0 - H_0)^{-1} Q H_B' \rangle + \langle H^{(6)} \rangle + \langle H^{(6)} \rangle.
\]

And now divergent terms are gathered together into the modified effective Hamiltonian \(H^{(6)} + H^{(6)}\).
The explicit form for the expectation value of the modified effective Hamiltonian can be written:

\[
\langle H^{(6)} \rangle + \langle H^{(6)} \rangle = \frac{\langle p^6 \rangle}{16m^5} + \frac{5\langle (E_1 + E_2)^2 \rangle}{32m^3} + \frac{9\langle p^4 V + V p^2 \rangle}{128m^4} + \frac{\pi \langle V (\rho_1 + \rho_2) \rangle}{2m^3} - \frac{5\langle V \rangle}{16m^2} - \frac{3\pi E_0 \langle (\rho_1 + \rho_2) \rangle}{4m^3} + \frac{5E_0^2 \langle V \rangle}{8m^3} - \frac{5E_0^2 \langle V \rangle \langle H_B \rangle}{16m^2} + \frac{2m}{\langle V \rangle \langle H_B \rangle}. \tag{20}
\]

The first five terms are divergent while the remaining part is finite. In Appendix B it is shown how the divergent terms may be transformed in a proper way to make them suitable for separation of divergent part, which then can be cancelled out. After summing up of all the terms of expression (20), one gets

\[
\langle H^{(6)} \rangle + \langle H^{(6)} \rangle = \frac{3E_0 \langle V \rangle}{4m^2} - \frac{5E_0^2 \langle V \rangle}{4m^2} - \frac{3\pi E_0 \langle (\rho_1 + \rho_2) \rangle}{4m^3} + \frac{\langle p^2 \rangle}{8m^3} + \frac{\langle V \rangle \langle H_B \rangle}{2m} + \frac{E_0^3}{2m^2}. \tag{21}
\]

All the expectation values in (21) are finite. Here \(E_0(R)\) is the ground-state energy of the two-centre problem (equation (1)) at a given bond length \(R\).
be treated separately in the usual way. The spin–orbit second-order iteration contribution does not contain a divergent part and can

4.4. Spin–orbit part

The spin–orbit second-order iteration contribution does not contain a divergent part and can be treated separately in the usual way

\[ \Delta E_{\text{so}}^{(6)} = (H_{\text{so}}^\infty Q(E_0 - H_0)^{-1} Q \ H_{\text{so}}^\infty). \]  \hspace{1cm} (22)

where

\[ H_{\text{so}}^\infty = \left( Z_1 \frac{[r_1 \times p]}{2m^2 r_1} + Z_2 \frac{[r_2 \times p]}{2m^2 r_2} \right) s. \]

For \( \sigma \)-states, \( \delta_\sigma \equiv 0 \), and without loss of generality we can consider that our first-order solution has a spin state \( s_z = 1/2 \), then the second-order spin–orbit contribution can be rewritten in terms of variables \( r_1 \) and \( r_2 \) as

\[ \Delta E_{\text{so}}^{(6)} = \frac{ir E^{-i\omega}}{4m^2} \left( \frac{Z_1}{r_1^3 r_2} \frac{\partial_{r_2}}{r_1^2 \partial_{r_1}} - \frac{Z_2}{r_1 r_2^3} \frac{\partial_{r_1}}{r_2^2 \partial_{r_2}} \right) \Psi_0 |(E_0 - H_0)^{-1}| \]

\[ \times \frac{ir E^{-i\omega}}{4m^2} \left( \frac{Z_1}{r_1^3 r_2} \frac{\partial_{r_2}}{r_1^2 \partial_{r_1}} - \frac{Z_2}{r_1 r_2^3} \frac{\partial_{r_1}}{r_2^2 \partial_{r_2}} \right) \Psi_0. \]  \hspace{1cm} (23)
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5. Results and conclusion

Equations (19), (21) and (23) have been evaluated numerically using the variational expansion (3) and (4).

In tables 1 and 2 the relativistic corrections of order $m\alpha^6$ for the ground state of electron for symmetric $Z_1 = Z_2 = 1$ (H$_2^+$ molecular ion) and asymmetric (the antiprotonic helium atom) $Z_1 = 2$ and $Z_2 = -1$ cases are presented as functions of bond length. The accuracy of obtained results for $\Delta E^{(6)}$ is estimated as all digits indicated in the tables. Figures 1 and 2
show the ‘effective’ potentials for these two cases. Dashed lines are the radial wavefunction for the ground and first vibrational S-states of H$_2^+$ and the (36, 34) state of the $^4\text{He}^+\bar{p}$ atom.

The last table gives a comparison of our calculations with the earlier ones, which demonstrate superiority of the newly obtained results. However, we want to draw attention to the approach of [18], which, to our opinion, is very promising and allows us to evaluate the $m\alpha^8$ order corrections as well using the same first-order perturbation wavefunction with a rather high accuracy. Presumably, the not very high precision of this particular calculation is connected with the Gaussian basis set, which is not very suitable for description of the zero-order and first-order solutions.

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Appendix A. Analytical evaluation of the matrix elements

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

$$\Gamma_{lm}(\alpha, \beta) = \int r_1^{l-1} r_2^{m-1} e^{-ar_1 - \beta r_2} \, dr_1 \, dr_2. \tag{A.1}$$

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

The function $\Gamma_{00}$ can be easily obtained as

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

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 the 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

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

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 [20]:

$$E_1(z) = \Gamma(0, z) = \int_{z}^{\infty} t^{-1} e^{-t} \, dt.$$
Appendix B. Relations between divergent matrix elements

In this section we will assume that $V$ is regularized in some or other way and $\rho = \rho_1 + \rho_2$ ($\Delta V = 4\pi \rho$) is a smooth function of space variables, a distribution of charge in space. The left- and right-hand side functions inside the brackets represent the same wavefunction $\Psi_0$. The solution of the Schrödinger equation (2). Then by using commutation relations and integration by parts one gets

\[ \langle V p^2 V \rangle = \langle V^2 p^2 \rangle - 4\pi \langle V (\rho_1 + \rho_2) \rangle + 2\langle V (\mathcal{E}_1 + \mathcal{E}_2) V \rangle. \]  
\[ \langle V p^2 V \rangle = \left(\langle (\mathcal{E}_1 + \mathcal{E}_2)^2 \rangle - 2\langle (\mathcal{E}_1 + \mathcal{E}_2) V \rangle + \langle p V^2 p \rangle \right). \]  
\[ 4\pi \langle V (\rho_1 + \rho_2) \rangle = -\langle (\mathcal{E}_1 + \mathcal{E}_2)^2 \rangle + 2\langle (\mathcal{E}_1 + \mathcal{E}_2) V \rangle. \]  

Subtracting equation (B.1c) from equation (B.1a), we have

\[ \langle V p^2 V \rangle = \langle \mathcal{E}_1 + \mathcal{E}_2 \rangle^2 + \langle p^2 p \rangle. \]  

then summing up (B.1b) and (B.1c) and taking into account (B.2a):

\[ 4\pi \langle V (\rho_1 + \rho_2) \rangle = -\langle (\mathcal{E}_1 + \mathcal{E}_2)^2 \rangle + \langle V^2 p^2 \rangle + \langle p V^2 p \rangle. \]  

From the last two formulae with a systematic use of

\[ p^2 \Psi_0 = 2m(E_0 - V)\Psi_0, \]

the final expressions for the divergent terms in equation (20) may be obtained:

\[ \frac{\langle p^4 \rangle}{16m^3} = \frac{\langle \mathcal{E}_1 + \mathcal{E}_2 \rangle^2}{4m^3} - \frac{\langle V \rangle^2}{2m^2} + \frac{3E_0 \langle V \rangle}{2m^2} - \frac{3E_0^2 \langle V \rangle}{2m^2} + \frac{E_0^3}{2m^2}. \]

\[ \frac{\langle p^4 + V p^4 \rangle}{128m^4} = -\frac{\langle \mathcal{E}_1 + \mathcal{E}_2 \rangle^2}{32m^3} + \frac{\langle V \rangle^3}{16m^2} - \frac{E_0 \langle V \rangle^2}{8m^2} + \frac{E_0^2 \langle V \rangle}{16m^2} + \frac{E_0^3}{8m^2}. \]

\[ \frac{\pi \langle V (\rho_1 + \rho_2) \rangle}{2m^3} = -\frac{\langle \mathcal{E}_1 + \mathcal{E}_2 \rangle^2}{8m^3} + \frac{\langle V \rangle^3}{4m^2} - \frac{E_0 \langle V \rangle^2}{4m^2} + \frac{E_0^2 \langle V \rangle}{8m^2}. \]

After summing up all the terms in (20) the regularization can be removed.

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