Spin-orbit corrections of order $ma^6$ to the fine structure of the (37,35) state in the $^4\text{He}^\ast \bar{p}$ antiprotonic helium atom

Vladimir I. Korobov*
Joint Institute for Nuclear Research, 141980 Dubna, Russia

Zhen-Xiang Zhong
State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics,
Chinese Academy of Science, 430071 Wuhan, China

(Received 11 August 2009; published 14 October 2009)

Precise numerical calculation of radiofrequency intervals between hyperfine sublevels of the (37,35) state of the antiprotonic helium-4 atom is presented. Theoretical consideration includes the QED corrections of order $ma^6$ to the electron spin-orbit interaction. Only the leading order contribution in the electron-to-antiproton and electron-to-$\alpha$ particle mass ratios is considered, so the $\alpha$ particle and antiproton are treated nonrelativistically. The effective Hamiltonian is derived using the formalism of the nonrelativistic quantum electrodynamics.

I. INTRODUCTION

The high precision spectroscopic measurement of the hyperfine structure (hfs) of the antiprotonic helium has twofold interest. First, it is expected that it may be a way to obtain improved value of the magnetic moment of an antiproton. The other point is that it can be a good benchmark for testing QED theoretical methods for the Coulomb three-body bound states to a high precision.

At present several theoretical calculations for the hyperfine structure of the (37,35) state of the $^4\text{He}^\ast \bar{p}$ atom have been performed [1–4]. Since all the results were obtained within the frames of the same Breit-Pauli approximation, the major difference in the obtained data was either due to numerical inaccuracy of the nonrelativistic solution or due to a difference in the choice of the physical constants. Still they were in a good agreement (within the error bars of the theoretical approximation) with the first experimental observation of the 13 GHz intervals [5].

Recently, the ASACUSA experiment has obtained new precise values for the two rf transitions of the (37,35) state in the $^4\text{He}^\ast \bar{p}$ atom [6,7] [the notation is shown on the schematic diagram of the (37,35) state on Fig. 1].

$$\tau_+ = 12\,896.641(63) \text{ MHz},$$

$$\tau_- = 12\,924.461(63) \text{ MHz}. \quad (1)$$

The difference between $\tau_+$ and $\tau_-$ is nearly proportional to the antiprotonic magnetic moment and has a value

$$\Delta \tau = 27.825(33) \text{ MHz}. \quad (2)$$

That should be compared with the theoretical prediction [3],

$$\tau_+ = 12\,986.35(69) \text{ MHz},$$

It is seen that the experimental error is more than one order of magnitude smaller and transitions have some systematic shift toward larger values. The Breit-Pauli approximation used so far is limited by the uncertainty of order $O(a^2)$ and higher order corrections should be included into consideration to achieve the similar accuracy as in the experiment.

The effective Hamiltonian of the hyperfine interaction may be written as (see details in [3])

$$H_{\text{eff}} = E_1(s_e \cdot L) + E_2(s_p \cdot L) + E_3(s_e \cdot s_p) + E_4(2L(L + 1)) \frac{\Delta s_e}{3} (s_e \cdot s_p - 3[s_e \cdot L(s_e \cdot L) + (s_e \cdot L)(s_p \cdot L)]) \quad (4)$$

To get improved values for the $\tau_+$ and $\tau_-$ transitions one needs to get contributions of the next to the leading order for the electron spin-orbit interaction coefficient $E_1$. It may be done within the framework of the nonrelativistic quantum electrodynamics (NRQED) formalism [8]. Some details of the derivation of the $ma^6$ order contributions may be found in [9].

FIG. 1. Schematic diagram of hyperfine sublevels of the (37,35) state of $^4\text{He}^\ast \bar{p}$ atom.

*korobov@theor.jinr.ru
II. CORRECTIONS OF ORDER $m\alpha^6$ TO THE EFFECTIVE
HAMILTONIAN OF THE FINE STRUCTURE

In what follows we use the following notations: $R_1, R_2, r$, and $P_1, P_2, p$, are coordinates and impulses of three particles in the center of mass frame, where subscript 1 stands for a helium nucleus and 2 for an antiproton. We also make use $r_i = r_i - R_i, i = 1, 2$ for coordinates of an electron with respect to one of the nuclei.

According to the NRQED the effective Hamiltonian includes the three interactions, which contribute to the electron spin-orbit term at the $m\alpha^6$ order. Two are relativistic corrections of order $v^2/c^2$ to the vertex functions for the spin-orbit and Fermi interactions (see [8]),

$$V_1 = e^2 \left( \frac{3\alpha_e}{8m_e^3} \frac{1}{q^3} \right) \left( \frac{r_i}{2r_i} \right)_i,$$

$$V_2 = -e^2 \left( \frac{1}{8m_e^3} \frac{1}{q^3} \right) \left( \frac{r_i}{2r_i} \right)_i,$$

Here $\alpha_e$ are the two-component Pauli matrices acting on the wave function of the electron.

The third is the seagull vertex interaction with one Coulomb and one transverse photon line,

$$V_3 = e^2 \left( \frac{3\alpha_e}{4m_e^3} \right) \left( \frac{1}{q^3} \right) \left( \frac{r_i}{2r_i} \right)_i + (1 \rightarrow 2).$$

The sources may be two different nuclei or may coincide.

To get a complete set of corrections one needs to take into account the second-order contribution as well,

$$\Delta E_A = 2\alpha^4\langle H_B | Q(E_0 - H_0)^{-1} Q | Z(r_i \times P_i) \rangle \frac{1}{m_i M_i r_i^3} \Delta s,$$

$$-2\alpha^6\langle H_B | Q(E_0 - H_0)^{-1} Q | Z(r_i \times P_i) \rangle \frac{1}{m_i M_i r_i^3} \Delta s,$$

where $Q$ is the projection operator on the subspace orthogonal to the wave function of the initial nonrelativistic Schrödinger solution and

$$H_B = -\frac{p_i^2}{2m_e} + \frac{\pi}{2m_e} [Z_i \delta(r_i) + Z_2 \delta(r_2)].$$

Radiative corrections (form factors of the electron) have already been included into consideration as contributions to the anomalous magnetic moment.

Transforming potentials $V_i$ to the coordinate space and atomic units one gets

$$V_1 = -e^2 \left( \frac{3Z_i}{16m_e^3} \right) \left( \frac{1}{r_i} \right) \left( \frac{r_i}{2r_i} \right)_i,$$

$$V_2 = e^2 \left( \frac{Z_i}{4m_e^3} \right) \left( \frac{1}{r_i} \right) \left( \frac{r_i}{2r_i} \right)_i.$$
For the intermediate states of the second-order iteration the similar variational expansion [Eq. (11)] with various basis lengths $N=520–960$ has been used.

IV. REDUCE A SINGULARITY IN THE SECOND-ORDER CONTRIBUTION

The $H_B$ operator in the second-order term [Eq. (7)] is too singular. It requires careful consideration because intermediate states should include functions with asymptotic behavior at small distances such as $\sim 1/r_1 (1/r_2)$. The usual regular trial functions would result in a very slow convergence of $\Delta E_A$

In order to smooth the perturbation and to reduce the singularity of the intermediate wave function we may use transformation

$$H'_B = H_B - (E_0 - H_0)U - U(E_0 - H_0).$$  \hspace{1cm} (13)

The delta-function singularity in $|H_B\Psi_0\rangle$ has the following structure:

$$H_B \Psi_0 = -\frac{1}{m_1^2} \left[ Z_1 \left( \frac{\mu_1}{m_e} - \frac{1}{2} \right) \pi \delta(r_1) + Z_2 \left( \frac{\mu_2}{m_e} - \frac{1}{2} \right) \pi \delta(r_2) \right] \Psi_0 + \cdots,$$  \hspace{1cm} (14)

where $1/\mu_1 = 1/m_e + 1/M_i$.

It is natural to take $U$ in the form $U = c_1/r_1 + c_2/r_2$. The coefficients $c_i$ may be obtained by substituting $U$ into the initial Schrödinger equation,

$$(E_0 - H_0) \left( \frac{c_1}{r_1} + \frac{c_2}{r_2} \right) = -\frac{2c_1}{\mu_1} \pi \delta(r_1) - \frac{2c_2}{\mu_2} \pi \delta(r_2) + \cdots.$$

Then comparing the latter expression with Eq. (14) one gets

$$c_1 = \frac{\mu_1 (2\mu_1 - m_e)}{4m_e^3} Z_1,$$

$$c_2 = \frac{\mu_2 (2\mu_2 - m_e)}{4m_e^3} Z_2.$$  \hspace{1cm} (15)

Thus the second-order term may be rewritten as follows:

$$\langle H_B | Q(E_0 - H_0)^{-1} Q | H_{SO} \rangle = \langle H'_B | Q(E_0 - H_0)^{-1} Q | H_{SO} \rangle + \langle U H_{SO} \rangle - \langle U \rangle | H_{SO} \rangle.$$

Matrix elements of $H'_B$ may be obtained directly from Eq. (13). Additional term to the effective Hamiltonian is expressed as

$$\langle H_m^{(6)} \rangle = \langle U H_{SO} \rangle - \langle U \rangle | H_{SO} \rangle = \left( \frac{c_1}{r_1} + \frac{c_2}{r_2} \right) | H_{SO} \rangle - \left( \frac{c_1}{r_1} + \frac{c_2}{r_2} \right) | H_{SO} \rangle.$$  \hspace{1cm} (17)

For the numerical evaluation of the second-order term from Eq. (16) we use the eight basis sets, where the first two approximate the regular part of the intermediate solution and the remaining six sets with growing exponents are introduced to reproduce behavior of the type $\ln(r_1) [\ln(r_2)]$ at small values of $r_1 (r_2)$. The particular variational parameters used are presented in Table I.

<table>
<thead>
<tr>
<th>Set</th>
<th>$[A_1,A_2]$</th>
<th>$[A'_1,A'_2]$</th>
<th>$[B_1,B_2]$</th>
<th>$[C_1,C_2]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>First</td>
<td>[66.6, 87.6]</td>
<td>[0.4, 5.2]</td>
<td>[0.00, 2.05]</td>
<td>[0.00, 0.87]</td>
</tr>
<tr>
<td>Second</td>
<td>[66.0, 75.4]</td>
<td>[0.0, 5.4]</td>
<td>[0.94, 5.70]</td>
<td>[0.00, 1.94]</td>
</tr>
<tr>
<td>Third</td>
<td>[66.0, 75.4]</td>
<td>[0.0, 5.4]</td>
<td>[5.00, 80.0]</td>
<td>[0.00, 0.10]</td>
</tr>
<tr>
<td>Fourth</td>
<td>[66.0, 75.4]</td>
<td>[0.0, 5.4]</td>
<td>[0.00, 0.20]</td>
<td>[2.00, 70.0]</td>
</tr>
<tr>
<td>Fifth</td>
<td>[66.0, 75.4]</td>
<td>[0.0, 5.4]</td>
<td>[90.0, 1000.0]</td>
<td>[0.00, 0.10]</td>
</tr>
<tr>
<td>Sixth</td>
<td>[66.0, 75.4]</td>
<td>[0.0, 5.4]</td>
<td>[0.00, 0.10]</td>
<td>[80.0, 800.0]</td>
</tr>
<tr>
<td>Seventh</td>
<td>[66.0, 75.4]</td>
<td>[0.0, 5.4]</td>
<td>[10^3, 10^{14}]</td>
<td>[0.00, 0.10]</td>
</tr>
<tr>
<td>Eighth</td>
<td>[66.0, 75.4]</td>
<td>[0.0, 5.4]</td>
<td>[0.00, 0.10]</td>
<td>[800.0, 10^4]</td>
</tr>
</tbody>
</table>

V. NUMERICAL CALCULATIONS

Matrix elements in Eqs. (9), (10a), (16), and (17) for the basis functions [Eq. (11)] of the exponential variational expansion were evaluated analytically using the recurrences derived in [12] with some modifications, which allowed us to improve stability. The generating functions $\Gamma_{-1,0,0}(\alpha, \beta, \gamma), \Gamma_{-1,-1,0}(\alpha, \beta, \gamma)$ were taken from [13]. What corresponds to the cutoff regularization of the integrals at $r_{1,2}=\rho$, where $\rho<1$?

For all vector operators the reduced matrix element is assumed. Here we present numerical values of some of the most complicated operators,

$$\left\langle \frac{p_x}{r_1} \right| 1 \right\rangle = 1.557 592 9,$$

$$\left\langle \frac{p_x}{r_2} \right| 2 \right\rangle = 2.245 924 3,$$

$$\left\langle \frac{p_x}{r_1} \right| 3 \right\rangle = 3272.7020,$$

$$\left\langle \frac{p_x}{r_2} \right| 4 \right\rangle = -3080.3879.$$  \hspace{1cm} (18)

$$\left\langle \frac{1}{r_2} \right| 5 \right\rangle = 205.832 72,$$

$$\left\langle \frac{1}{r_1} \right| 6 \right\rangle = 1391.5321,$$

$$\left\langle \frac{r_1 \times r_2}{r_1^3 r_2^3} \right| 7 \right\rangle = 551.654 20,$$

$$\left\langle \frac{r_1 \times r_2}{r_1^3 r_2^3} \right| 8 \right\rangle = 551.433 28.$$  \hspace{1cm} (19)
TABLE II. Convergence of the second-order contribution matrix elements for the spin-orbit interaction.

<table>
<thead>
<tr>
<th>$n_1$</th>
<th>$n_2$</th>
<th>$n_3$</th>
<th>$\frac{[r_1 \times p_1]}{r_1^3}$</th>
<th>$\frac{[r_1 \times P_1]}{r_1^3}$</th>
<th>$\frac{[r_2 \times p_3]}{r_2^3}$</th>
<th>$\frac{[r_2 \times P_3]}{r_2^3}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>20</td>
<td>20</td>
<td>0.2883781</td>
<td>680.02999</td>
<td>0.5135404</td>
<td>−1204.595</td>
</tr>
<tr>
<td>20</td>
<td>20</td>
<td>20</td>
<td>0.2411901</td>
<td>624.7925</td>
<td>0.4875501</td>
<td>−1177.070</td>
</tr>
<tr>
<td>40</td>
<td>20</td>
<td>20</td>
<td>0.2242844</td>
<td>573.8206</td>
<td>0.4899458</td>
<td>−1192.019</td>
</tr>
<tr>
<td>60</td>
<td>20</td>
<td>20</td>
<td>0.2536075</td>
<td>633.29499</td>
<td>0.5022857</td>
<td>−1194.613</td>
</tr>
<tr>
<td>60</td>
<td>40</td>
<td>20</td>
<td>0.2322982</td>
<td>526.5736</td>
<td>0.4881029</td>
<td>−1187.319</td>
</tr>
<tr>
<td>60</td>
<td>40</td>
<td>40</td>
<td>0.2847268</td>
<td>714.1212</td>
<td>0.4849738</td>
<td>−1160.058</td>
</tr>
<tr>
<td>80</td>
<td>40</td>
<td>40</td>
<td>0.2812069</td>
<td>716.9230</td>
<td>0.4696484</td>
<td>−1159.465</td>
</tr>
</tbody>
</table>

\[
\langle H_B^0 \rangle |Q(E_0 - H_0)^{-1}Q | \frac{[r_1 \times p_1]}{r_1^3} \rangle = 0.2812, \\
\langle H_B^0 \rangle |Q(E_0 - H_0)^{-1}Q | \frac{[r_2 \times p_3]}{r_2^3} \rangle = 0.4696, \\
\langle H_B^0 \rangle |Q(E_0 - H_0)^{-1}Q | \frac{[r_1 \times P_1]}{r_1^3} \rangle = 717.0, \\
\langle H_B^0 \rangle |Q(E_0 - H_0)^{-1}Q | \frac{[r_2 \times P_3]}{r_2^3} \rangle = -1160. \quad (20)
\]

It is worthy to say that the second-order iteration, even after reduction of the singularity, still reveals slow convergence. In Table II we present results of numerical calculations for various sets of basis functions. The results depend very little on increase of the first and second basis sets (see Table I), which represent regular behavior. The following notation has been used in Table II: $n_1$ are a number of basis functions for third and fourth sets, $n_2$ are for fifth and sixth sets, etc. As is seen from Table II, no more than two digits may be accepted with confidence as convergent. However, the increase of the basis sets leads to numerical instability, which we attribute to very large angular momentum of the state ($L = 35$) that makes the recursion used for analytic evaluation of the matrix elements to be too long and unstable for large exponents. The octuple precision has been used in these calculations and still it was not enough to provide necessary stability.

VI. RESULTS AND DISCUSSION

Summing up the contributions from Eqs. (7), (9), (10a), and (10b) we obtain the $ma^6$ order contribution to the electron spin-orbit interaction,

\[
\Delta E_1 = -0.000 \ 030(4) \times 10^{-7} \text{ a.u.} \quad (21)
\]

Thus a new value for the $E_1$ coefficient would be

\[
E_1 = -0.552 \ 563(4) \times 10^{-7} \text{ a.u.,} \quad (22)
\]

where the uncertainty is primarily due to slow convergence of the second-order iteration.

Using this new value for the $E_1$ coefficient and keeping $E_2 - E_4$ as in [3] one may solve effective Hamiltonian (4) and get updated theoretical values for transition frequencies,

\[
\tau_+ = 12 \ 897.0(1)/(3) \text{ MHz}, \\
\tau_\gamma = 12 \ 924.9(1)/(3) \text{ MHz}, \\
\Delta \tau = 27.897(0)/(3) \text{ MHz.} \quad (23)
\]

The first error indicates the numerical uncertainty of present calculations, while the second one is an estimate of the theoretical uncertainty due to yet uncalculated higher order terms. As it should be $\Delta \tau$ does not change its value comparing with previous calculations [3]. The values of $\tau_+$ and $\tau_\gamma$ leap over the experimental result and overestimate ones if we take the numerical error as a measure of uncertainty. Still in theory we need to include into consideration effects of the next order in $\alpha$, which contain terms of order $(\alpha^3 \ln \alpha) E_1$ and are of the magnitude of the discrepancy.

It is worth noting here that the obtained value of $\Delta E_1$ is unexpectedly small. That explains rather good agreement of the experiment with the results of the Breit-Pauli approximation.

In order to get the improved value for $\Delta \tau$ one needs to perform a complete calculation of all the contributions of order $ma^6(m/M)$, which provides corrections to the remaining coefficients, $E_2 - E_4$, in the effective hfs Hamiltonian (4). This work is in progress now.

ACKNOWLEDGMENTS

The support of the Russian Foundation for Basic Research under Grants No. 08-02-00341 and No. 09-02-91000-ASF is gratefully acknowledged.
