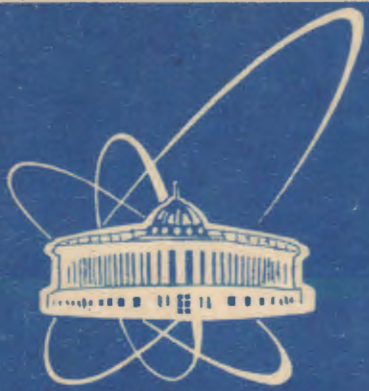

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ENERGY-LEVEL SPLITTING IN ANTIPROTONIC HELIUM ATOMS

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1 Introduction

Metastable antiprotonic helium atoms $^{3,4}He\bar{p}e$ have been discovered in experiments on the delayed annihilation of antiprotons in helium media [1], [2]. Analogous long-lived systems were observed in experiments with negative kaons [3] and pions [4]. The discussion of the theoretical calculations on antiprotonic helium atoms and related topics can be found in [5].

The precise measurement of transition energies of antiprotonic helium atoms in recent experiments on the laser-induced resonant annihilation [6], [7], [8] invokes the theoretical description of energy spectra with comparable accuracy. Such a description of energy spectra requires that minor effect of relativistic and QED interactions and the coupling with the continuous spectrum should be taken into account. The relativistic corrections of an order of α^2 ($\alpha = e^2/\hbar c$ – fine structure constant) to the pure Coulomb interaction are the most important and should be firstly considered. Next in line are QED corrections to energies of higher orders in α.

Since the contribution to energies from the relativistic interactions depends on the antiproton mass, charge and magnetic moment, the comparison of precise calculations and measurements of the energy spectra can be used for determining the antiproton properties. This knowledge is significant in testing the fundamental symmetry principles. The detailed discussion of this problem can be found in [9].

The spin-dependent part of the relativistic interactions gives rise to splitting of energy levels, and each single transition turns into a multiplet. Sufficiently large distances between lines in the multiplet can be measured experimentally. It is worthwhile to mention that the resolution in current experiments is about 10GHz and without much difficulty can be improved to 1GHz [10]. As it will be discussed below, due to the interaction with electron spin, antiprotonic helium energy levels split into two multiplets and the interaction with nuclei spins provides a minor splitting into each multiplet. Values of the former large splitting are presented in this report.

The relativistic interaction in antiprotonic helium atoms is described in the next section, and in section 3 the method of calculation of the level splitting is discussed. Numerical results are presented in section 4; outlook and discussion, in the last section.

2 Relativistic interaction

For each pair of particles i,j in the three-body system the relativistic correction of an order of α^2 to the pure Coulomb two-body potential can be described by the Breit interaction of the form

$$U_{ij} = -\alpha^2 Z_i Z_j \Big(\frac{\pi}{2}(m_i^{-2} + m_j^{-2})\delta(\mathbf{r}_{ij}) + \frac{1}{2m_i m_j r_{ij}}(\mathbf{p}_i\mathbf{p}_j + r_{ij}^{-2}\mathbf{r}_{ij}(\mathbf{r}_{ij}\mathbf{p}_i)\mathbf{p}_j) + \frac{\mu_i}{2m_i^2 r_{ij}^3}[\mathbf{r}_{ij}\mathbf{p}_i]\mathbf{s}_i - \frac{\mu_j}{2m_j^2 r_{ij}^3}[\mathbf{r}_{ij}\mathbf{p}_j]\mathbf{s}_j + \frac{1}{m_i m_j r_{ij}^3}(\mu_j[\mathbf{r}_{ij}\mathbf{p}_i]\mathbf{s}_j - \mu_i[\mathbf{r}_{ij}\mathbf{p}_j]\mathbf{s}_i) - \frac{\mu_j\mu_j}{m_i m_j}\big(r_{ij}^{-3}\mathbf{s}_i\mathbf{s}_j - 3(\mathbf{r}_{ij}\mathbf{s}_i)(\mathbf{r}_{ij}\mathbf{s}_j) - \frac{8\pi}{3}\mathbf{s}_i\mathbf{s}_j\delta(\mathbf{r}_{ij})\big)\Big), \quad (1)$$

where $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, $\mathbf{r}_i, \mathbf{p}_i, \mathbf{s}_i, m_i, Z_i, \mu_i$ are the radius-vector, momentum, spin, mass, charge and magnetic moment (in units $e\hbar/2m_ic$) of particle i. Here and below atomic units ($\hbar = e = m_e = 1$) are used. The correction to the kinetic energy of an order of α^2 for each particle i is

$$\Delta T_i = -\frac{\alpha^2}{8}\frac{p_i^4}{m_i^3} \quad (2)$$

Full relativistic correction H_r of an order of α^2 to the three-body nonrelativistic Hamiltonian is a sum of U_{ij} for all pairs of particles and ΔT_i for all particles

$$H_r = \sum_i \Delta T_i + \sum_{i>j} U_{ij}. \quad (3)$$

Using expressions $U_{ij}, \Delta T_i$ in eq. (3), particles momenta $\mathbf{p}_i$ will be taken in the center of mass frame of the three-body system [11]. Below, for definiteness helium nucleus, antiproton and electron will be enumerated as particles $1,2,3$, respectively. Relative coordinates $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$, $\boldsymbol{\rho} = \mathbf{r}_3 - \mathbf{r}_1$, corresponding momenta $\mathbf{p} = -i\nabla_{\mathbf{r}}$, $\mathbf{q} = -i\nabla\boldsymbol{\rho}$ and angular momenta $\mathbf{l} = [\mathbf{rp}]$, $\boldsymbol{\lambda} = [\boldsymbol{\rho}\mathbf{q}]$ will be used to simplify notation.

The interaction H_r, given in (3), conserves the sum $\mathbf{J} = \mathbf{L} + \sum_i \mathbf{s}_i$ of the total angular momentum $\mathbf{L} = \mathbf{l} + \boldsymbol{\lambda}$ and particle spins $\mathbf{s}_i$. Each level of the nonrelativistic Hamiltonian splits into four and eight sublevels for $^4He\bar{p}e$ and $^3He\bar{p}e$ systems, respectively. Due to very small mass ratios $m_3/m_1, m_3/m_2$, the largest contribution to the energy splitting comes from the interaction with the electron spin $\mathbf{s}_3$. Taking into consideration only terms responsible for the splitting in (2), (3), this part of relativistic interaction can be written as follows:

$$H_s = \alpha^2\Big(\frac{1}{\rho^3}\boldsymbol{\lambda}\mathbf{s}_3 + \frac{1}{2|\mathbf{r}-\boldsymbol{\rho}|^3}([\mathbf{r}-\boldsymbol{\rho},\mathbf{q}]\mathbf{s}_3) - \frac{1}{m_2|\mathbf{r}-\boldsymbol{\rho}|^3}([\mathbf{r}-\boldsymbol{\rho},\mathbf{p}]\mathbf{s}_3) + \frac{2}{m_1\rho^3}([\boldsymbol{\rho},\mathbf{p}]\mathbf{s}_3)\Big) \quad (4)$$

While the last two terms in (5) are inversely proportional to the heavy particle masses $m_{1,2}$, their contribution to the energy splitting is nevertheless comparable to the contribution from the first two terms due to the following reasons. The small mass factor is compensated in part due to the large angular momentum $l \sim L$ of heavy particles. At the same time, only small components of the wave function corresponding to the nonzero electron angular momenta $\lambda \neq 0$ lead to the nonzero splitting value from the first two terms in (5).

3 Level splitting

The interaction H_s, given in (5), conserves the sum $\mathbf{j} = \mathbf{L} + \mathbf{s}_3$ of the total angular momentum $\mathbf{L} = \mathbf{l} + \boldsymbol{\lambda}$ and electron spin $\mathbf{s}_3$ and splits each level into two sublevels, corresponding to the eigenvalues $j = L \pm 1/2$. The part of the interaction depending on heavy particle spins removes the remaining degeneracy and splits each $j = L \pm 1/2$ sublevel further into two or four levels for the $^4He\bar{p}e$ and $^3He\bar{p}e$ systems, respectively. Values of this secondary splitting are much smaller in comparison with the splitting, arisen due to the interaction with the electron spin (5). By this reason only calculation of major splitting will be presented in this report.

The nonrelativistic Hamiltonian of the antiprotonic helium atom is

$$H = -\frac{1}{2\mu}\Delta_{\mathbf{r}} - \frac{1}{2\mu_1}\Delta_{\boldsymbol{\rho}} - \frac{1}{m_1}\nabla_{\mathbf{r}}\cdot\nabla_{\boldsymbol{\rho}} - \frac{2}{r} - \frac{2}{\rho} + \frac{1}{|\mathbf{r}-\boldsymbol{\rho}|}, \quad (5)$$

where $1/\mu = 1/m_1 + 1/m_2$, $1/\mu_1 = 1/m_1 + 1/m_3$. The nonrelativistic wave function ψ_{LN} and energy E_{LN} is the N-th solution and eigen-energy of the Schrödinger equation

$$(H - E_{LN})\psi_{LN} = 0 \quad (6)$$

for the total angular momentum L. Since the splitting is small in comparison with energy differences between states of different L values, the energy shift

Δ_{LN} can be found in the first order of perturbation theory over H_s

$$\Delta_{jLN} = (\Psi_{jLN}|H_s|\Psi_{jLN}\rangle, \qquad (7)$$

where Ψ_{jLN} is the vector production of ψ_{LN} and spin function describing the dependence of the electron spin.

Since the interaction H_s (5) is of the form $H_s = \mathbf{A}s_3$, the energy shift Δ_{jLN} can be expressed

$$\Delta_{jLN} = \frac{j(j+1) - L(L+1) - 3/4}{2\sqrt{L(L+1)(2L+1)}}\langle\psi_{LN}||\mathbf{A}||\psi_{LN}\rangle, \qquad (8)$$

where the notation $\langle\cdot||\cdot||\cdot\rangle$ stands for the reduced matrix element. Level splitting $\Delta E_{LN} = \Delta_{L+1/2LN} - \Delta_{L-1/2LN}$ is a difference of shifts (8) for the $j = L \pm 1/2$.

Due to smallness of the relativistic interaction, radiative transitions proceed only between states of the same j. By this reason, in experiment each spectral line of the transition from the state L_iN_i to state L_fN_f is to be split into a doublet with the interline distance $\Delta\nu = \Delta E_{L_iN_i} - \Delta E_{L_fN_f}$.

4 Numerical results

The variational method, described in [12], was applied to determine eigenfunctions and eigenenergies of the Schrödinger equation (6). The set of simple variational trial functions of the form

$$\chi^{LM}_{nkl\lambda i}(\mathbf{r},\boldsymbol{\rho}) = \mathcal{Y}^{LM}_{l\lambda}(\hat{\mathbf{r}},\hat{\boldsymbol{\rho}})r^{l+i}\rho^{\lambda}exp(-a_nr - b_k\rho), \qquad (9)$$

where $\mathcal{Y}^{LM}_{l\lambda}(\hat{\mathbf{r}},\hat{\boldsymbol{\rho}})$ are bispherical harmonics of angular variables, was used in the calculations.

Splitting values ΔE_{LN} have been calculated as described above (7), (8) by using variational nonrelativistic wave functions. Up to 600 trial functions (reftrial) containing up to 15 bispherical harmonics were used in these calculations. Nonlinear parameters a_n, b_k were taken the same as in the previous variational calculation of energies and radiative transition rates [12].

Splitting values for a number of states of the $^{3,4}He\bar{p}e$ systems in the range of experimentally observed values of the total angular momentum L are presented in Table 1.

Table 1. Splitting values ΔE_{LN} (10^{-6}au) of the lowest levels in the $^{3,4}He\bar{p}e$ systems.

$^4He\bar{p}e$						
N	L=32	L=33	L=34	L=35	L=36	L=37
1	-1.10	-1.15	-1.15	-1.14	-1.12	-1.09
2	-1.12	-1.09	-1.08	-1.07	-1.04	-1.00
3	-1.01	-1.02	-1.00	-0.98	-0.94	-0.90
4		-0.94	-0.94	-0.90	-0.86	-0.82
5			-0.93	-0.90	-0.84	-0.81
$^3He\bar{p}e$						
N	L=31	L=32	L=33	L=34	L=35	L=36
1	-1.20	-1.16	-1.19	-1.19	-1.18	-1.14
2	-1.14	-1.19	-1.15	-1.12	-1.08	-1.04
3	-1.08	-1.06	-1.05	-1.04	-1.00	-0.98
4		-0.97	-0.92	-0.86	-0.85	-0.81

As it follows from expression (5), the form of the wave function at small interparticle distances is the most important in evaluating the integral (7). Convergence of the calculated splitting provides a few per cent relative accuracy. It is worthwile to mention that due to the variational method of calculation the accuracy is better for the large L and small N states. It is impossible to trace the convergence in the case of short lived states due to a small multipolarity $\Delta l < 3$ of the Auger decay. This problem is closely connected with a large natural width of these states which exceeds significantly a splitting value. Also, the variational procedure meets some difficulties in describing the short range behavior of the wave function for the large enough N states, especially in the $^3He\bar{p}e$ system. These are reasons to omit the above–mentioned cases in Table 1.

The last two terms in eq. (5) describe the interaction of the electron magnetic moment with the magnetic field of heavy particles. These terms give rise to the largest contribution to the energy–level splitting. For better understanding the splitting dependence on L, N this contribution is presented in Table 2 for the $^4He\bar{p}e$ system. The contribution to the energy–level splitting from the first two terms in (5) are of the opposite sign and much smaller in magnitude. Nevertheless, decreasing in this contribution with increasing L compensates the L dependence of the last two terms in eq. (5) and provides a very slow dependence of the total splitting ΔE_{LN} on L.

Table 2. Contribution of the last two terms in eq. (5) to the energy–level splitting ΔE_{LN} (10^{-6}au) in the $^4He\bar{p}e$ system.

N	L=32	L=33	L=34	L=35	L=36	L=37
1	-1.41	-1.43	-1.40	-1.37	-1.34	-1.28
2	-1.39	-1.34	-1.30	-1.27	-1.22	-1.16
3	-1.26	-1.24	-1.20	-1.15	-1.10	-1.04
4		-1.14	-1.11	-1.06	-1.00	-0.94
5			-1.10	-1.06	-0.98	-0.95

5 Discussion

Due to almost exact conservation of the j value in the radiative transition the spectral line splitting will be found as a difference of ΔE_{LN} presented in Table 1. Most appropriate for the experimental measurement are the favoured transitions between states of the same N, which have the largest radiative rates [12]–[14]. However, the calculated splitting values are almost independent of L for a given N, and it is not plausible to resolve such a small difference in splitting for the favoured transitions. For this reason, the experimental proposal for the near future [10] is aimed at searching for the splitting in unfavoured transitions $(L, N) \to (L-1, N+2)$.

In order to measure splitting in experiments on the laser–induced resonant annihilation the initial state will be long–lived. This is provided by the condition that the multipolarity of the Auger decay for this state is $\Delta l = 4$. The next condition is that the natural width of the short–lived final state will be smaller than the splitting value, and the multipolarity of the Auger decay for this state will be $\Delta l = 3$. The spectral line splitting for a number of suitable transitions is presented in Table 3. These values are of an order of the experimentally measurable value ~1GHz.

Comparing the splitting values for the $^4He\bar{p}e$ and $^3He\bar{p}e$ systems one can mention in the $^4He\bar{p}e$ case a slower decreasing in ΔE_{LN} with increasing N. As it is clear from Table 3, this isotopic effect is also conserved for the spectral line splitting $\Delta\nu$.

Table 3. Spectral line splitting $\Delta\nu = \Delta E_{L_iN_i} - \Delta E_{L_fN_f}$ (GHz) for the transitions $E_{L_iN_i} \to E_{L_fN_f}$ in the $^{3,4}He\bar{p}e$ systems.

$^4He\bar{p}e$		$^3He\bar{p}e$	
$L_iN_i \to L_fN_f$	$\Delta\nu$	$L_iN_i \to L_fN_f$	$\Delta\nu$
33,1→32,3	-0.92	32,1→31,3	-0.53
34,1→33,3	-0.86	33,1→32,3	-0.86
34,2→33,4	-0.91	33,2→32,4	-1.22
35,2→34,4	-0.88	34,2→33,4	-1.35
35,3→34,5	-0.34		

The following considerations can be used to understand qualitatively the L, N–dependence of the energy–level splitting. Contribution to splitting from the interaction of the electron magnetic moment with the magnetic field of heavy particles is described by the last two terms in the splitting interaction H_s (5). This contribution is proportional to the relative momentum of heavy particles $\mathbf{p}$.One can consider that the motion of heavy particles is approximately the same as in a hydrogen–like atom and momentum p is inversely proportional to the angular momentum L. This is the reason for increasing this contribution with decreasing L, as presented in Table 2. The contribution from the first two terms in the splitting interaction H_s is connected with the electron rotation and proportional to the small component of the wave function arising due to polarization of an electron by $\bar{p}$. With decreasing L the antiproton moves to a region of increasing electron density and the polarization increases. In such a way contributions to the energy–level splitting from the last two terms in H_s and remaining part of splitting interaction are of opposite signs and level off the dependence of the total splitting ΔE_{LN} on L.

One can consider quasiclassically that the antiproton orbit became more stretched with increasing N at fixed total angular momentum. By this reason all the terms of the splitting interaction H_s decrease with encreasing L and provide the N dependence presented in Tables 1, 3.

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