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FINE AND HYPERFINE STRUCTURE
OF ANTIPROTONIC HELIUM

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1 Introduction

The recently discovered metastable states of the antiprotonic helium atoms [1, 2, 3] are of significant interest for both the experimentalists developing high precision laser spectroscopy methods and the theorists working on few-body problems. The phenomenon of delayed annihilation of antiprotons in helium seems to be qualitatively well understood within the Condo model [4]; the observed laser resonance wavelengths are interpreted in this model as E1-transitions in the exotic three-body system pHe^+ (referred to also as “atomcule”), stimulated by a laser tuned at the resonance frequency. This model will only be accepted, however, when the theoretical calculations of the energy spectrum of the atomcule agree with the experimental values within the very small experimental error. Until recently this was not the case since the results of some authors [3, 5] disagreed by as much as 1 nm , although the latest results of Puzynin *et al* [6] and especially, of Korobov [7] seem to have drastically reduced this discrepancy.

Of course, further improving of the accuracy of the numerical methods used for solving the three-body Coulomb problem is crucial, but also important now becomes the use of a realistic model for the atomcule which would account for the higher order QED corrections to the Coulomb interaction potential. Of particular interest was commonly expected to be the fine and hyperfine splitting of the Coulomb levels that might be partially responsible for the discrepancy between experiment and the pure Coulomb theory, so we decided first to calculate the spin interaction corrections and to leave all other effects - such as vacuum polarization and relativistic shift of the energy levels, corrections due to the interaction with the external laser field etc. - for later times. In what follows we report our first numerical results.

2 Outline of the theoretical approach

The leading order QED effects in few-body bound systems are described by means of the Breit Hamiltonian. As long as we restrict

ourselves to the evaluation of only the fine and hyperfine splitting of the nonrelativistic levels, we have kept the terms involving the particle spin operators $\vec{s}_i, i = 1, 2, 3$, and neglected all the spin-independent terms; we also have neglected the electromagnetic structure of the antiproton and the helium nucleus, but we did keep the terms involving particle magnetic moments $\mu_i, i = 1, 2, 3$ [8]. Thus, the perturbation Hamiltonian H_{int} took the form (in units $\hbar = c = 1$):

$$\begin{aligned}
H_{int} &= \alpha^2 (V_{12} + V_{13} + V_{23}) \quad (1) \\
V_{12} &= \frac{Z_2(2\mu_1 - Z_1)}{2M_1^2} \frac{1}{r_{21}^3} (\vec{r}_{21} \times \vec{P}_1) \cdot \vec{s}_1 - \frac{Z_2\mu_1}{M_1M_2} \frac{1}{r_{21}^3} (\vec{r}_{21} \times \vec{P}_2) \cdot \vec{s}_1 \\
V_{23} &= \frac{Z_2(2\mu_3 - Z_3)}{2M_3^2} \frac{1}{r_{23}^3} (\vec{r}_{23} \times \vec{P}_3) \cdot \vec{s}_3 - \frac{Z_2\mu_3}{M_2M_3} \frac{1}{r_{23}^3} (\vec{r}_{23} \times \vec{P}_2) \cdot \vec{s}_3 \\
V_{13} &= - \left(\frac{Z_1\mu_3}{M_3m_{13}} \vec{s}_3 + \frac{Z_3\mu_1}{M_1m_{13}} \vec{s}_1 \right) \frac{1}{r_{13}^3} (\vec{r}_{13} \times \vec{p}_{13}) \\
&\quad + \frac{Z_1Z_2}{2} \left(\frac{1}{M_3^2r_{13}^3} (\vec{r}_{13} \times \vec{P}_3) \cdot \vec{s}_3 - \frac{1}{M_1^2r_{13}^3} (\vec{r}_{13} \times \vec{P}_1) \cdot \vec{s}_1 \right) \\
&\quad - \frac{2\mu_1\mu_3}{3M_1M_3} 4\pi r_{13} \delta(r_{13}).
\end{aligned}$$

Here $Z_i, \vec{R}_i, \vec{P}_i$ and M_i denote the charge, position vector, momentum and mass of the i -th particle, $i=1,2,3$; $m_{ij} = M_iM_j/(M_i + M_j)$, $\vec{r}_{ij} = \vec{R}_j - \vec{R}_i$, $\vec{p}_{ij} = (M_i\vec{P}_j - M_j\vec{P}_i)/(M_i + M_j)$. We denote the antiproton, helium nucleus and the electron as particles 1,2 and 3, respectively.

We used as zeroth order approximation the nonrelativistic wave functions of the atomcule obtained in the adiabatic approach

$$\Psi^{vIM}(\vec{r}, \vec{R}) = \sum_{i,m} \chi_{im}^{vI}(R) \varphi_{im}(\xi, \eta; R) D_{mM}^I(\Phi, \Theta, \phi), \quad (2)$$

where \vec{r} and \vec{R} are Jacobi coordinates:

$$\vec{R} = \vec{R}_2 - \vec{R}_1, \quad \vec{r} = \vec{R}_3 - \frac{1}{2}(\vec{R}_1 + \vec{R}_2)$$

Φ, Θ and R are spherical coordinates of \vec{R} ; ξ, η and ϕ - prolate spheroidal coordinates of \vec{r} ; $\varphi_{im}(\xi, \eta; R)$ - Coulomb spheroidal basis functions [9], and $D_{mM}^l(\Phi, \Theta, \phi)$ are Wigner functions.

We further restricted ourselves - within the so called *one-level approximation* - to only the first term of the expansion in the R.H.S. with $m = 0$ (neglecting, among others, all π and higher terms).

The matrix elements of H_{int} are expressed in terms of integrals of products of the functions φ_{im} and χ_{im}^{vJ} over the variables ξ, η, R ; in our calculation we used the numerical values of φ_{im} and χ_{im}^{vJ} , obtained in [6].

3 Numerical results: discussion and perspectives

The nonrelativistic eigenstates of the three-body Coulomb problem are labeled with the orbital and principal quantum numbers l and $n = l + v + 1$, v being the vibrational quantum number. Taking into account the spin interaction H_{int} (1) requires two more quantum numbers - the total spin s and the total angular momentum J . Any of the nonrelativistic levels (n, l) , $l > 0$ splits into 4 sublevels ($s = 0, J = l$), ($s = 1, J = l$), ($s = 1, J = l - 1$) and ($s = 1, J = l + 1$), separated by quantities of the order of $10^{-5} eV$. One could further expect that the wavelength of the transition between two Coulomb states of the three-body $\bar{p}^4 He^+$ system, $(n, l) \rightarrow (n', l')$, $l' = l - 1$ will split into $4 \times 4 = 16$ components according to the initial and final values of the additional quantum numbers $(s, J) \rightarrow (s', J')$. As a matter of fact, a part of these transitions are strictly forbidden, four of the hyperfine components with $J' = J - 1, s' = s$ clearly dominate (in what follows they will be referred to as dominating or main components) and the others involve a suppression factor of order $O(J^{-2k})$, $k = |\Delta J - \Delta l|$. Among the transitions suppressed by a factor $1/4J^2 \sim 10^{-3} - 10^{-4}$ only two - $(s = 1, J = l) \rightarrow (s = 1, J' = l + 1)$ and $(s = 1, J = l - 1) \rightarrow (s = 0, J' = l')$ - have a significant separation of the energy levels; we shall not be interested in the remaining transitions which either are too

strongly suppressed or lie too close to the main components to be distinguished of them.

Tables 1 and 2 present our numerical results for the shift of the wavelength of the four main and two suppressed transitions among the hyperfine components of the levels of antiproton helium atoms that undergo the E1-transition $(n, l) \rightarrow (n', l')$ with $l' = l - 1$ for $30 \leq l \leq 40$. The tables cover the cases $n' = n - 1$ and $n' = n + 1$, respectively. (Note that the rate of the transitions with $n' = n - 1$ exceeds the rate for the case $n' = n + 1$ by two orders of magnitude [3]). The fine and hyperfine shift of the main components is much below the present accuracy of the spectroscopical measurements $\sim 10^{-3} nm$ [3] and can be neglected. What could in principle be observed are the two suppressed transitions discussed above, the wavelengths of which are separated from the main lines by more than one laser wavelength width [3]; unfortunately the overall probability for these suppressed transitions (referred to as "suppression factor" in the Tables) is of the order of 10^{-3} .

The accuracy of our results on the fine and hyperfine splitting of the transitions wavelengths is estimated to be of the order of 20%. The main uncertainty comes from the one-level approximation adopted earlier. While the missing π -terms in the expansion of Eq. 2 contribute to the nonrelativistic energy values by quantities of order 10^{-4} [7, 6], the contribution of the spin-orbit interaction term

$$\frac{Z_2(2\mu_3 - Z_3)}{2M_3^2} \frac{1}{r_{23}^3} (\vec{r}_{23} \times \vec{P}_3) \cdot \vec{s}_3$$

(that vanishes in the σ -terms approximation) is expected to be of the order of 20% of the contribution of the leading spin-orbit term

$$\frac{Z_2\mu_3}{M_2M_3} \frac{1}{r_{23}^3} (\vec{r}_{23} \times \vec{P}_2) \cdot \vec{s}_3.$$

Note that the contribution of the higher order QED corrections that are not included in the spin interaction Hamiltonian of Eq. 1 does not exceed 1%. The numerical inaccuracy of the nonrelativistic wave functions is much smaller and its impact on the splitting

Table 1: Fine and hyperfine structure of the transitions $(n,l) \rightarrow (n-1,l-1)$ of $\bar{p}^4\text{He}^+$

$(n,l) \rightarrow (n',l')$	Coulomb values [nm]	Splitting of the transition wavelengths, [10^{-4} nm]						suppr. factor $\times 10^3$
		Dominating				Suppressed		
		$s=0$		$s=1$		$\Delta s=0$	$\Delta s=-1$	
		$J=l$	$J=l$	$J=l-1$	$J=l+1$	$\Delta J=1$		
32,31→31,30	265.0	.00	.00	.00	.03	-1.95	-1.98	.26
33,31→32,30	297.6	.00	.00	.00	.00	-2.35	-2.38	.26
34,31→33,30	334.4	.03	.03	.00	.00	-2.81	-2.87	.26
35,31→34,30	375.7	.06	.06	.03	.00	-3.33	-3.36	.26
36,31→35,30	422.3	.09	.06	.03	-.06	-3.94	-4.00	.26
33,32→32,31	296.4	.00	.00	.00	.00	-2.47	-2.50	.25
34,32→33,31	333.0	.00	.03	.00	.00	-2.93	-2.96	.25
35,32→34,31	374.4	.03	.06	.03	.00	-3.48	-3.51	.25
36,32→35,31	421.0	.06	.06	.03	-.03	-4.09	-4.15	.25
37,32→36,31	473.6	.09	.06	.03	-.06	-4.79	-4.88	.25
34,33→33,32	331.6	.00	.03	.00	.00	-3.05	-3.08	.23
35,33→34,32	373.0	.00	.03	.03	.00	-3.63	-3.69	.23
36,33→35,32	419.7	-.06	.06	.03	-.03	-4.30	-4.33	.23
37,33→36,32	472.4	-.09	.06	.06	-.06	-5.04	-5.07	.23
38,33→37,32	531.7	-.12	.12	.12	-.12	-5.86	-5.92	.23
35,34→34,33	371.4	-.03	.03	.03	-.03	-3.81	-3.85	.22
36,34→35,33	418.2	-.06	.06	.03	-.03	-4.52	-4.55	.22
37,34→36,33	471.2	-.09	.09	.09	-.06	-5.31	-5.34	.22
38,34→37,33	530.9	-.12	.06	.06	-.12	-6.16	-6.23	.22
39,34→38,33	597.9	-.18	.18	.12	-.12	-7.08	-7.14	.22
36,35→35,34	416.6	-.06	.06	.03	-.03	-4.73	-4.76	.21
37,35→36,34	469.9	-.09	.09	.09	-.09	-5.55	-5.62	.21
38,35→37,34	530.1	-.18	.18	.12	-.12	-6.47	-6.53	.21
39,35→38,34	597.8	-.18	.18	.12	-.12	-7.51	-7.57	.21
40,35→39,34	673.4	-.24	.24	.18	-.24	-8.61	-8.67	.21
37,36→36,35	468.4	-.06	.09	.09	-.06	-5.80	-5.86	.20
38,36→37,35	529.2	-.18	.18	.12	-.12	-6.77	-6.84	.20
39,36→38,35	597.7	-.18	.24	.24	-.12	-7.87	-7.87	.20
40,36→39,35	674.4	-.24	.31	.24	-.18	-9.03	-9.09	.20
41,36→40,35	759.6	-.37	.31	.31	-.31	-10.31	-10.38	.20

Table 1 (continued)

38,37→37,36	528.2	-.18	.18	.12	-.12	-7.14	-7.20	.19
39,37→38,36	597.7	-.18	.24	.24	-.18	-8.30	-8.36	.19
40,37→39,36	675.8	-.31	.37	.31	-.24	-9.52	-9.58	.19
41,37→40,36	762.5	-.43	.37	.31	-.37	-10.93	-10.99	.19
42,37→41,36	857.8	-.43	.49	.43	-.43	-12.33	-12.39	.19
39,38→38,37	597.9	-.18	.31	.24	-.18	-8.79	-8.79	.18
40,38→39,37	677.4	-.31	.31	.31	-.24	-10.13	-10.13	.18
41,38→40,37	766.1	-.43	.37	.37	-.37	-11.60	-11.66	.18
42,38→41,37	863.7	-.55	.49	.43	-.43	-13.06	-13.12	.18
43,38→42,37	969.7	-.67	.61	.61	-.67	-14.59	-14.65	.18
40,39→39,38	679.6	-.37	.37	.31	-.31	-10.68	-10.74	.17
41,39→40,38	770.6	-.49	.43	.37	-.43	-12.27	-12.33	.17
42,39→41,38	870.8	-.55	.61	.49	-.49	-13.85	-13.92	.17
43,39→42,38	979.6	-.61	.73	.67	-.61	-15.50	-15.56	.17
44,39→43,38	1096.5	-1.10	1.22	1.22	-.98	-16.72	-16.72	.17
41,40→40,39	776.2	-.49	.55	.49	-.43	-13.00	-13.06	.16
42,40→41,39	879.5	-.61	.67	.61	-.61	-14.77	-14.77	.16
43,40→42,39	991.8	-.73	.79	.79	-.73	-16.54	-16.60	.16
44,40→43,39	1112.1	-1.10	1.22	1.10	-1.10	-18.07	-18.07	.16
45,40→44,39	1239.6	-1.95	2.08	1.83	-1.95	-17.94	-18.07	.16

Table 2: Fine and hyperfine structure of the transitions $(n,l) \rightarrow (n+1,l-1)$ of $\bar{p}^4\text{He}^+$.

$(n,l) \rightarrow (n',l')$	Coulomb values [nm]	Splitting of the transition wavelengths, [10^{-3}nm]						suppr. factor $\times 10^3$
		Dominating				Suppressed		
		s=0	s=1			$\Delta s=0$	$\Delta s=-1$	
		$J=l$	$J=l$	$J=l-1$	$J=l+1$	$\Delta J=l$		
32,31→33,30	343.0	-15	-18	-15	-15	3.17	3.17	.26
33,31→34,30	392.9	-24	24	21	-21	3.91	3.91	.26
34,31→35,30	450.5	31	34	27	-27	4.85	4.85	.26
33,32→34,31	394.9	21	24	24	-24	4.15	4.15	.25
34,32→35,31	453.7	31	34	34	-31	5.16	5.19	.25
35,32→36,31	521.8	43	43	43	-37	6.35	6.41	.25
34,33→35,32	457.0	34	34	31	-34	5.49	5.52	.23
35,33→36,32	526.9	43	43	43	-43	6.84	6.84	.23
36,33→37,32	607.8	61	55	55	-61	8.36	8.36	.23
35,34→36,33	532.4	49	55	55	-43	7.39	7.39	.22
36,34→37,33	615.9	67	67	61	-61	9.09	9.09	.22
37,34→38,33	712.5	79	79	79	-79	11.17	11.17	.22
36,35→37,34	624.9	67	73	67	-67	9.89	9.89	.21
37,35→38,34	725.2	85	92	85	-85	12.21	12.21	.21
38,35→39,34	840.7	110	116	110	-110	14.89	14.95	.21
37,36→38,35	739.6	98	104	104	-92	13.43	13.43	.20
38,36→39,35	860.7	128	128	128	-122	16.42	16.42	.20
39,36→40,35	998.6	153	165	159	-153	20.08	20.08	.20
38,37→39,36	883.5	140	140	140	-134	18.31	18.31	.19
39,37→40,36	1029.3	171	183	171	-171	22.34	22.34	.19
40,37→41,36	1193.0	220	220	220	-208	26.98	26.98	.19
39,38→40,37	1065.0	208	208	208	-195	25.15	25.15	.18
40,38→41,37	1239.3	244	256	256	-232	30.52	30.52	.18
41,38→42,37	1431.4	293	293	293	-281	36.13	36.13	.18
40,39→41,38	1293.9	293	305	293	-281	34.91	34.91	.17
41,39→42,38	1499.1	330	354	354	-330	41.50	41.50	.17
42,39→43,38	1719.8	403	415	415	-391	48.22	48.22	.17
41,40→42,39	1580.1	391	415	415	-391	48.22	48.22	.16
42,40→43,39	1815.3	464	476	476	-464	55.91	55.91	.16
43,40→44,39	2061.3	659	684	684	-659	62.01	62.01	.16

of our numerical values for the *shift* of the transition wavelengths can be neglected; of course, more accurate numbers for the *transition wavelengths themselves* (referred to as “Coulomb values” in the Tables) are highly desirable.

The obvious very next step should be the use of more precise wave functions of the $p\ ^1He^+$ atomcule that go beyond the one-level expansion in Eq. 2. Still more important for the comparison of theory with experiment seem to be the spin-independent QED and relativistic corrections to the energy levels of the atomcule, that we expect to be dominated by the vacuum polarization correction to the Coulomb potential and eventually the relativistic corrections to the kinetic energy. The calculation of these effects in other exotic three-body systems [10, 11] shows that their contribution may exceed the spin corrections by order of magnitudes.

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В данной работе представлены результаты численных расчетов тонкого и сверхтонкого расщепления уровней энергии экзотического атома $\bar{p}\text{He}^+$ для возбужденных вращательных состояний антипротона для значений орбитального момента $30 \leq J \leq 40$. Вычисления выполнены в одноуровневом адиабатическом приближении кулоновской задачи трех тел с использованием релятивистского трехчастичного гамильтониана, описывающего спиновые эффекты в приближении однофотонного обмена. Хотя погрешность наших результатов порядка нескольких процентов, мы ясно показываем, что спиновым эффектом можно пренебречь при присписывании квантовых чисел начальным и конечным состояниям экспериментально обнаруженных E1-переходов [1,2,3]. Мы также указываем на возможность экспериментального измерения тонкого расщепления уровней системы $\bar{p}\text{He}^+$, стимулируя один из подавленных переходов, резонансная частота которых отделена от главного пика на расстояние, превышающее ширину лазерной линии.

Работа выполнена в Лаборатории вычислительной техники и автоматизации ОИЯИ.

Препринт Объединенного института ядерных исследований. Дубна, 1995

We present the numerical results for the fine and hyperfine splitting of the energy levels of the exotic atom $\bar{p}\text{He}^+$ in angular excited states with antiproton orbital momentum in the range $30 \leq J \leq 40$. Calculations have been performed in the one-level adiabatic approximation, in the framework of the adiabatic representation of the Coulomb three-body problem and with the use of a relativistic three-body Hamiltonian describing the spin effects in the one-photon-exchange approximation. Though uncertainty of our results is of the order of a few percent, we clearly demonstrate that the spin effects can be neglected when ascribing the quantum numbers to the initial and final states of the experimentally observed E1-transitions [1,2,3]. We also point on the possibility of experimentally measuring the fine splitting of the levels of $\bar{p}\text{He}^+$ by stimulating one of the suppressed transitions, the resonance frequency which is separated from the main peak by a gap that exceeds the width of the laser line.

The investigation has been performed at the Laboratory of Computing Techniques and Automation, OIYI.

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