Hyperfine structure of metastable states in $^3He^+\bar{p}$ atom

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For the metastable states of antiprotonic helium atoms, $^3He^+\bar{p}$, the fine and hyperfine splittings of energy levels are calculated within the framework of the Breit-Pauli Hamiltonian. The latter represents the α^2 order relativistic corrections to the nonrelativistic energy. Results include as well the leading α^3 order contribution due to the anomalous magnetic moment of electron. The final relative accuracy of the hyperfine intervals is estimated to be about 5×10^{-5}.

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I. INTRODUCTION

During the past ten years, the experimental accuracy in spectroscopic measurements of transition lines between metastable states in an antiprotonic helium atom has been increased [1,2] from few parts per million (ppm) to several parts per billion (ppb) [3] and further improvement to a sub-ppb lever is expected (see a review [4] for details). A one ppb level means that the experimental results become sensitive to the uncertainty in the (anti)proton/electron mass ratio [5]. At this level of precision, information about sublevels of the fine and hyperfine structure is crucial for proper determination of the "central" spin-averaged transition frequency.

Furthermore, the microwave experiments for direct measurement of the hyperfine structure (HFS) in antiprotonic helium-4 atoms have been carried out recently [6]. The aim of these experiments is to improve the value of the magnetic moment of an antiproton known so far with rather poor accuracy of 0.3%. In a forthcoming series of experiments, it is expected to obtain precise data on the hyperfine intervals both in helium-4 and helium-3 atoms.

So far, an extensive study of the HFS of the helium-4 states has been carried out in Refs. [7–9]. For the helium-3 case, however, only one publication is available [10], where results have been obtained with the use of the coupled rearrangement channel variational method of Gaussian type. The purpose of this work is to present an independent and extended calculation of the hyperfine structure in $^3He^+\bar{p}$ atoms.

In what follows, atomic units are used throughout.

II. VARIATIONAL WAVE FUNCTION

In our calculations, we use the exponential variational expansion, which has been discussed in various ways in a variety of works [11–13]. Details and strategy of particular choice of the variational nonlinear parameters and basis structure that has been adopted in the present work can be found in Ref. [14] and those typical for the antiprotonic helium atoms in Ref. [15].

Briefly, the wave function for a state with a total orbital angular momentum L and of a total spatial parity $\pi=(-1)^L$ is expanded as follows:

$$\Psi(\mathbf{r}_1,\mathbf{r}_2)=\sum_{l_1+l_2=L}\mathcal{Y}^{l_1l_2}_{LM}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)G^{L\pi}_{l_1l_2}(r_1,r_2,r_{12}),$$

$$G^{L\pi}_{l_1l_2}(r_1,r_2,r_{12})=\sum_n C_n e^{-\alpha_n r_1-\beta_n r_2-\gamma_n r_{12}}, \quad (1)$$

where $\mathbf{r}_1$ is a position vector of an antiproton and $\mathbf{r}_2$ is a position vector of an electron with respect to a nucleus (helion); parameters in exponents are generated in a pseudorandom way,

$$\alpha_n=\left[\left\lfloor\tfrac{1}{2}n(n+1)\sqrt{p_\alpha}\right\rfloor(A_2-A_1)+A_1\right],$$

$$\beta_n=\left[\left\lfloor\tfrac{1}{2}n(n+1)\sqrt{p_\beta}\right\rfloor(B_2-B_1)+B_1\right],$$

$$\gamma_n=\left[\left\lfloor\tfrac{1}{2}n(n+1)\sqrt{p_\gamma}\right\rfloor(C_2-C_1)+C_1\right]. \quad (2)$$

Here, $\lfloor x\rfloor$ denotes the fractional part of x, and p_α, p_β, or p_γ are some prime numbers. The advantage of these simple generators of pseudorandom numbers is the ability to reproduce results of previous variational calculations.

However, when exponents α_n, β_n, and γ_n are real, the method reveals slow convergence for molecular type Coulomb systems. In order to cure this problem, one may switch to complex exponents and then use instead of (1) the following expansion:

$$\Psi(r_1,r_2,r_{12})=\sum_{n=1}^{N}\{C_n\,\mathrm{Re}[e^{-\alpha_n r_1-\beta_n r_2-\gamma_n r_{12}}] + D_n\,\mathrm{Im}[e^{-\alpha_n r_1-\beta_n r_2-\gamma_n r_{12}}]\}. \quad (3)$$

For the antiprotonic helium metastable states, the variational solution with this basis set provides an accuracy of about 10^{-10}–10^{-12} a.u. for the nonrelativistic energies at moderate basis lengths of $N=1000$–1200.

III. BREIT-PAULI HAMILTONIAN

The leading correction to the nonrelativistic energy is the α^2 order relativistic correction determined by the Breit-Pauli Hamiltonian. It is derived in many different ways (see, for example, Ref. [16,17]) for a system with a number of particles greater than two. For a composite particle, the finite size electromagnetic structure plays an important role, the

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TABLE I. Coefficients of the effective Hamiltonian (in 10^{-12} a.u.).

(n,l)	E_1	E_2	E_3	E_4	E_5	E_7	E_8	E_9
(31,30)	−75 333.77	2013.787	−1021.587	−76 680.56	−514 257.6	−11.550 23	0.948 421	−0.541 187
(32,31)	−72 874.55	1588.638	−819.5040	−70 659.35	−553 210.9	−11.354 01	0.910 356	−0.406 011
(33,31)	−68 427.31	1388.983	−719.5835	−62 325.06	−614 396.2	−11.763 11	0.918 418	−0.356 565
(34,31)	−63 637.48	1214.753	−631.6302	−54 389.84	−675 656.5	−11.957 38	0.916 723	−0.313 097
(33,32)	−70 128.41	1251.272	−657.8301	−64 469.23	−595 018.3	−11.110 67	0.871 443	−0.305 411
(34,32)	−65 320.74	1091.152	−575.9888	−56 257.42	−65 8792.1	−11.357 13	0.872 926	−0.267 535
(35,32)	−60 294.43	951.0382	−503.7652	−48 631.25	−722 061.3	−11.395 05	0.865 490	−0.234 114
(36,32)	−55 171.96	829.4708	−440.6018	−41 700.88	−783 188.0	−11.232 35	0.848 660	−0.204 885
(34,33)	−67 068.28	982.6191	−527.7282	−58 150.81	−639 716.2	−10.813 81	0.831 493	−0.230 048
(35,33)	−61 911.97	854.4058	−460.6073	−50 159.09	−705 419.5	−10.894 49	0.826 243	−0.200 937
(36,33)	−56 646.49	742.8777	−401.6934	−42 902.35	−769 369.8	−10.772 88	0.811 598	−0.175 379
(37,33)	−51 422.86	646.4982	−350.3799	−36 473.79	−830 140.4	−10.471 61	0.787 425	−0.153 102
(35,34)	−63 672.35	768.2345	−422.5347	−51 752.25	−687 233.6	−10.456 88	0.790 641	−0.173 283
(36,34)	−58 210.15	666.0303	−367.5496	−44 102.20	−754 036.6	−10.372 59	0.778 332	−0.150 889
(37,34)	−52 769.96	577.8712	−319.6835	−37 328.64	−817 666.0	−10.101 16	0.756 864	−0.131 378
(38,34)	−47 508.82	502.3901	−278.3759	−31 480.82	−876 809.4	−9.676 596	0.727 296	−0.114 521

interaction of such a particle with electromagnetic field is discussed in Ref. [18]. In a more recent paper by Kinoshita and Nio [19], it is shown using the nonrelativistic QED theory how the electromagnetic structure of nuclei can be incorporated into the Breit-Pauli Hamiltonian in a proper way.

The spin dependent part of the Hamiltonian for a system of particles of spin 1/2 has the following form:

$$H_B = -\frac{e^2}{c^2}\sum_{j\neq i}\frac{Z_i Z_j c_S^{(j)}[\mathbf{r}_{ij}\times\mathbf{p}_j]\mathbf{s}_j}{2m_j^2 r_{ij}^3} - \frac{e^2}{c^2}\sum_{i>j}\frac{Z_i Z_j (c_F^{(i)}[\mathbf{r}_{ij}\times\mathbf{p}_j]\mathbf{s}_i - c_F^{(j)}[\mathbf{r}_{ij}\times\mathbf{p}_i]\mathbf{s}_j)}{m_i m_j r_{ij}^3} + \sum_{i>j}\left\{\left[\frac{\boldsymbol{\mu}_i\boldsymbol{\mu}_j}{r_{ij}^3} - 3\frac{(\boldsymbol{\mu}_i\mathbf{r}_{ij})(\boldsymbol{\mu}_j\mathbf{r}_{ij})}{r_{ij}^5}\right] - \frac{8\pi}{3}\boldsymbol{\mu}_i\boldsymbol{\mu}_j\delta(\mathbf{r}_{ij})\right\}. \tag{4}$$

Here $\boldsymbol{\mu}_i=(c_F^{(i)}Z_i/2m_i c)\boldsymbol{\sigma}_i$ is an operator of magnetic moment and coefficients c_F and c_S are defined as

$$c_F^{(i)} = 1 + \kappa_i,$$

$$c_S^{(i)} = 1 + 2\kappa_i,$$

where κ_i is an anomalous magnetic moment of a particle.

In the calculations presented below, the following values of physical constants have been adopted: $\kappa_h=-4.184\,153$, $\kappa_{\bar{p}}=1.792\,847\,337$, and $a_e=1.159\,652\,186\times10^{-3}$.

IV. EFFECTIVE HAMILTONIAN

The effective Hamiltonian, which arises from Eq. (4), has a form of spin-spin and spin-orbital angular momentum interactions

$$\begin{aligned} H_{\text{eff}} = {} & E_1(\mathbf{L}\cdot\mathbf{s}_e) + E_2(\mathbf{L}\cdot\mathbf{s}_{\bar{p}}) + E_3(\mathbf{L}\cdot\mathbf{s}_h) + E_4(\mathbf{s}_e\cdot\mathbf{s}_{\bar{p}}) \\ & + E_5(\mathbf{s}_e\cdot\mathbf{s}_h) + E_6(\mathbf{s}_{\bar{p}}\cdot\mathbf{s}_h) + E_7\{2L(L+1)(\mathbf{s}_1\cdot\mathbf{s}_2) \\ & - 3[(\mathbf{L}\cdot\mathbf{s}_1)+(\mathbf{L}\cdot\mathbf{s}_2)]\} + E_8\{2L(L+1)(\mathbf{s}_1\cdot\mathbf{s}_3) \\ & - 3[(\mathbf{L}\cdot\mathbf{s}_1)+(\mathbf{L}\cdot\mathbf{s}_3)]\} + E_9\{2L(L+1)(\mathbf{s}_2\cdot\mathbf{s}_3) \\ & - 3[(\mathbf{L}\cdot\mathbf{s}_2)+(\mathbf{L}\cdot\mathbf{s}_3)]\}. \end{aligned} \tag{5}$$

It is scalar and couples eight states with the same J_z. In fact, it is a block diagonal matrix with two one-dimensional blocks for the states with $J=L\pm3/2$ and two three-dimensional blocks for the states with $J=L\pm1/2$. The matrix elements of the Hamiltonian (5) can be easily obtained by using the algebra of angular momentum, the necessary formulas can be found, for example, in Ref. [20].

Coefficients E_i are obtained numerically by evaluating operators from (4), which depend on the spatial degrees of freedom. An analytical integration of the matrix elements is then reduced to integrals of a form

$$\Gamma_{lmn}(\alpha,\beta,\gamma) = \int\int r_1^l r_2^m r_{12}^n e^{-\alpha r_1-\beta r_2-\gamma r_{12}} dr_1 dr_2 dr_{12},$$

where some of the indices (l,m,n) may acquire negative values up to −4. The integrals in this case are divergent, but in operators they are encountered in such combinations that the final expression is finite, thus the divergent terms are canceled out. In our calculation, we follow the numerical scheme described in Ref. [21]. In a more transparent way, the

TABLE II. Fine and hyperfine splitting (in MHz) of energy levels for the states of the $^3He^+\bar{p}$ atom.

(n,l)	$+++$	$++-$	$+-+$	$+--$	$-++$	$-+-$	$--+$	$---$
(31,30)	−8244.32	−8542.09	−6502.11	−6788.68	8852.29	8334.72	7187.64	6681.28
(32,31)	−8312.40	−8560.39	−6503.83	−6742.89	8899.94	8485.12	7044.81	6638.92
(33,31)	−7953.77	−8192.15	−6027.76	−6258.06	8569.25	8229.10	6428.77	6096.71
(34,31)	−7560.84	−7790.95	−5531.16	−5753.47	8222.34	7946.91	5782.51	5514.87
(33,32)	−8335.16	−8546.72	−6451.11	−6655.35	8914.61	8588.80	6859.44	6540.94
(34,32)	−7927.29	−8134.27	−5925.46	−6125.45	8548.73	8287.67	6191.68	5937.61
(35,32)	−7496.75	−7698.74	−5395.39	−5590.13	8180.26	7974.22	5506.65	5307.86
(36,32)	−7053.94	−7249.99	−4878.36	−5066.22	7821.35	7660.59	4820.24	4667.66
(34,33)	−8307.74	−8493.34	−6341.56	−6520.84	8891.49	8643.06	6624.01	6381.90
(35,33)	−7849.11	−8033.31	−5769.39	−5947.08	8490.19	8297.06	5904.09	5717.48
(36,33)	−7377.36	−7558.59	−5208.59	−5382.45	8097.73	7950.13	5180.35	5040.12
(37,33)	−6906.66	−7083.00	−4679.06	−4846.51	7729.48	7617.98	4471.78	4369.17
(35,34)	−8225.21	−8392.92	−6173.20	−6335.01	8826.40	8645.20	6331.89	6156.58
(36,34)	−7717.53	−7885.42	−5561.50	−5722.73	8393.16	8257.99	5563.50	5435.00
(37,34)	−7209.07	−7374.66	−4979.90	−5137.37	7982.75	7883.88	4808.25	4717.51
(38,34)	−6715.16	−6876.00	−4447.97	−4598.58	7610.65	7539.09	4085.96	4024.62

generating functions [say, $\Gamma_{-4,0,0}(\alpha,\beta,\gamma)$, etc.] have been obtained in Ref. [22].

Results of calculation for the states of the antiprotonic helium atom, $^3He^+\bar{p}$, are presented in Table I. Coefficient E_6 is defined by the expectation value $\langle\delta(\mathbf{r}_{h\bar{p}})\rangle$, which is formally nonzero for the three-body system. But due to a large orbital momentum of an antiprotonic orbital, $L>30$, it is negligibly small and is not shown in the Table I.

V. SPIN FUNCTIONS

We adopt the following coupling scheme for spins: $\mathbf{F}=\mathbf{L}+\mathbf{s}_e$, $\mathbf{G}=\mathbf{F}+\mathbf{s}_h$, and $\mathbf{J}=\mathbf{G}+\mathbf{s}_{\bar{p}}$, since operators $\mathbf{F}$ and $\mathbf{G}$ provide good approximate quantum numbers.

A general hyperfine substate can be expressed as

$$\Psi(JJ_z)=\sum_{L_z+\zeta_e+\zeta_h+\zeta_{\bar{p}}=J_z} C_{L_z\zeta_e\zeta_h\zeta_{\bar{p}}}(|\upsilon LL_z\rangle|s_e\zeta_e\rangle|s_h\zeta_h\rangle|s_{\bar{p}}\zeta_{\bar{p}}\rangle). \tag{6}$$

States corresponding to the adopted coupling of angular momenta are expressed in terms of the Clebsch-Gordan coefficients

$$|\upsilon LFGJJ_z\rangle=\sum_{\zeta_e,\zeta_h,\zeta_{\bar{p}}} C^{LFGJJ_z}_{L_z\zeta_e\zeta_h\zeta_{\bar{p}}}\times(|\upsilon LL_z\rangle|s_e\zeta_e\rangle|s_h\zeta_h\rangle|s_{\bar{p}}\zeta_{\bar{p}}\rangle), \tag{7}$$

where

$$C^{LFGJJ_z}_{L_z\zeta_e\zeta_h\zeta_{\bar{p}}}=C^{FF_z}_{LL_zs_e\zeta_e}C^{GG_z}_{FF_zs_h\zeta_h}C^{JJ_z}_{GG_zs_{\bar{p}}\zeta_{\bar{p}}}.$$

For this basis set of spin functions, the off-diagonal matrix elements of the effective Hamiltonian are small. It means that the spin function (6) of a hyperfine substate is approximately described by the appropriate function defined by (7). Still, the exact solution is a mixture of states of the same J.

Owing to the property that the effective Hamiltonian is about diagonal, it is convenient to introduce the following notation. Say, the state with approximate quantum numbers $F=L+s_e$ and $G=F-s_h$ and total angular momentum $J=G-s_{\bar{p}}$ will be denoted by $|+--\rangle$ and similarly for other states.

VI. RESULTS

Numerical results for the energy shift of the sublevel relative to the "spin-averaged" energy are presented in Table II. They are obtained by direct numerical diagonalization of the effective (8×8) Hamiltonian (5) discussed above.

It is worth noting that the calculations presented here involve the consideration of only the leading order terms to the fine and hyperfine structure of the states of the antiprotonic helium atom, $^3He^+\bar{p}$. Since neither corrections of relativistic nature $(Z\alpha)^2$, nor radiative ones of order $\alpha(Z\alpha)$ have been included here, the relative accuracy of obtained hyperfine intervals is limited by about 50 ppm. The numerical errors are estimated to be smaller.

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