Variational calculation of antimprotonic helium atoms

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Abstract

A few per cent fraction of antiprotons stopped in helium survives for an enormous time (up to tens of microseconds) in comparison with the usual lifetime \((10^{-12}\text{s})\) of these particles in matter. The explanation is that antiprotons are captured in the metastable antimprotonic helium atoms \(^3\bar{\text{He}}^\text{pe}\) carrying an extremely large total angular momentum \(L \sim 30 - 40\). Initial populations, level lifetimes and very precise values of the transition energies were obtained in experiments on the resonant laser-induced annihilation. Analogous long-lived systems were observed in experiments with negative kaons and pions.

The purpose of this report is to present the results of calculation of eigenenergies, radiative transition rates, energy-level splitting due to relativistic interactions and Auger decay rates of antimprotonic helium atoms within the variational approach.
1 Introduction

The lifetime of negatively charged heavy particles (such as $\pi^-$, $K^-$, $\bar{p}$) stopped in matter would be about $10^{-12}$s due to nuclear absorption after exotic-atom formation. Recently it has been found that a small fraction (a few per cent) of kaons [1], pions [2] and antiprotons [3], [4] stopped in helium media survive for an enormous time (up to tens of microseconds for antiprotons). The reason for this unusual behavior is the formation of a metastable three-body system consisting a helium nucleus, an electron and a negative heavy particle. The prediction of these systems were made as early as thirty years ago by Condo [5] to explain a considerable difference of pion lifetimes in liquid helium and hydrogen. Later on, this qualitative prediction was supported by the variational calculations of Russell [6]. One can mention also the first calculation of the antiprotonic helium atom using the Born-Oppenheimer approximation [7]. Since antiprotons are stable and lifetime of an antiprotonic helium is the largest among these exotic systems, the experimental data concern mainly the antiprotonic helium atom. The modern experiments on the resonant laser-induced annihilation [8, 9] have initiated thorough investigations of these unusual systems. Initial populations, level lifetimes, and very precise values of the transition energies (with a relative accuracy $< 10^{-5}$) have been obtained using this remarkable method.

The antiprotonic helium can be considered as a counterpart of the usual helium atom with one electron replaced by an antiproton. A large angular momentum $L \sim (\mu/m_3)^{1/2}$ ($\mu$ is the reduced mass of the antiproton–nucleus subsystem and $m_3$ is the electron mass) provides that the antiproton-nucleus and electron-nucleus distances are approximately equal. At the same time, this system can be considered as an exotic diatomic molecule, where one nucleus is negatively charged [10].

While there is a number of processes destroying the antiprotonic helium atom, the following considerations explain its very long lifetime. The most part of an extremely large total angular momentum $L \sim 35 - 40$ belongs to the pair of heavy particles and annihilation of an antiproton is inhibited by a large centrifugal barrier. The Auger decay is inhibited due to sufficiently large values ($\lambda_0 \geq 4$) of the angular momentum of an outgoing electron. Usual mechanism of the de-excitation by the Stark mixing is not appropriate for the three-body system due to the lack of degeneracy. The collisional de-excitation by surrounding $He$ atoms is suppressed due to the screening of an antiproton by the electron in an antiprotonic helium. The only remaining de-excitation mechanism is multistep dipole radiative transitions, whose rates of each step are of order $\mu s^{-1}$. The discussion of theoretical calculations on antiprotonic helium atoms and related topics can be found in [11].

After the formation of the antiprotonic helium its time evolution is determined by the processes of radiative transition and Auger decay. The precise description of energy spectra requires to take into account the minor effect of relativistic interactions. The spin-dependent part of relativistic interactions gives rise to splitting of energy levels and sufficiently large splitting values can be measured experimentally. The direct variational method provides a possibility in the framework of one approach to calculate eigenenergies, energy-level splitting due to relativistic interactions, radiative transition rates and Auger decay rates of antiprotonic helium atoms. The results of these calculations are presented
and discussed in this report. The isotopic effect is considered by comparison of the calculated properties of $^4\text{He}^{-}\bar{e}$ and $^3\text{He}^{-}\bar{e}$.

2 Variational method

The nonrelativistic Hamiltonian of the antiprotonic helium atom in the triangular coordinates is

$$
H = -\frac{1}{2\mu} \Delta_r - \frac{1}{2\mu_1} \Delta_\rho - \frac{1}{m_1} \nabla_r \cdot \nabla_\rho - \frac{2}{r} - \frac{2}{\rho} + \frac{1}{|r - \rho|},
$$

(1)

where $1/\mu = 1/m_1 + 1/m_2$, $1/\mu_1 = 1/m_1 + 1/m_3$ and $m_1, r_1, m_2, r_2, m_3, r_3$ are masses and coordinates of the helium nucleus, antiproton and electron, respectively. Apart from the triangular coordinates $r = r_2 - r_1$, $\rho = r_3 - r_1$, the Jacobi coordinates $r = r_2 - r_1$, $\rho_1 = r_3 - (m_1 r_1 - m_2 r_2)/(m_1 + m_2)$, corresponding momenta $p = -i\nabla_r$, $q = -i\nabla_\rho$, $q_1 = -i\nabla_\rho_1$ and angular momenta $l = [r p]$, $\lambda = [\rho q]$, $\lambda_1 = [\rho_1 q_1]$ will be used to simplify the notation.

Since antiprotonic helium atoms are unstable against the decay to the $\text{He}^{-}\bar{e} + e$ channel, the variational method cannot be directly applied to the calculation of energies and wave functions. Therefore, according to [12] the approximate Hamiltonian $H_{LN} = P_{LN} H P_{LN}$ which is the projection of the Hamiltonian $H$ onto the closed-channel subspace was constructed to calculate the $N$-th energy level $E_{LN}$ of the system for the total angular momentum $L$. Explicitly $P_{LN}$ is constructed as a projector onto the subspace of eigenfunctions of relative angular momenta $l, \lambda$ (or $l, \lambda_1$), belonging to a limited set of $l, \lambda$ (or $l, \lambda_1$) eigenvalues. While using the Jacobi coordinates this set is defined by the condition $l > l_0$, where $l_0$ is the largest pair angular momentum satisfying the inequality $\varepsilon_{l_0} < E_{LN}$ and $\varepsilon_{l_0}$ is the energy of the hydrogen-like ion $^3\text{He}^-\bar{e}$ with the angular momentum $l_0$. If the triangular coordinates are used, this set can be defined by the condition $\lambda < \lambda_0$, where $\lambda_0$ is the smallest angular momentum satisfying the inequality $\varepsilon_{l - \lambda_0} < E_{LN}$. By definition, $\lambda_0$ is also a multipolarity of the Auger transition, i.e. the smallest angular momentum of the outgoing electron. These conditions describe the natural way to provide the approximate Hamiltonian $H_{LN}$ to have at least $N$ eigenvalues below the boundary of the continuous spectrum and the variational method can be applied to solve the eigenvalue problem for $N$ lowest states of $H_{LN}$.

It is worthwhile to mention that the $l = L$ projection is the main part of the wave function and the contribution of $l \neq L$ projection rapidly decreases with increasing $|l - L|$. For this reason the approximate Hamiltonian $H_{LN}$ provides an accurate calculation of energies $E_{LN}$ and wave functions $\Psi_{LN}$ for an metastable states ($\lambda_0 \geq 4$) of antiprotonic helium atoms. In fact, the described conditions on $l, \lambda$ are more restrictive than necessary for an application of the variational method. Practically the accuracy of calculation can be improved taking into account $\lambda > \lambda_0$ (or $l < l_0$ in the case of the Jacobi coordinates) components of the wave function. While using these components a convergence of the calculated values with increasing the number of trial functions will be investigated to provide the reliable results.
3 Energy levels

The variational method described in the previous section was applied to determine eigenfunctions and eigenenergies of the equation

\[(H_{LN} - E_{LN})\Psi_{LN} = 0.\] (2)

A set of simple variational trial functions of the form

\[\chi_{nkl\lambda}(r, \rho) = Y_{LM}^{l\lambda}(\hat{r}, \hat{\rho}) r^l + i \rho^\lambda \exp(-a_n r - b_k \rho),\] (3)

where \(Y_{LM}^{l\lambda}(\hat{r}, \hat{\rho})\) are bispherical harmonics of angular variables, was used in the calculations. It is essential that \(Y_{LM}^{l\lambda}(\hat{r}, \hat{\rho})\) are eigenfunctions of \(l, \lambda\) and this form of trial functions allows the easy application of the projection method described in Section 2.

Up to 1000 trial functions (3) containing up to 25 bispherical harmonics were used in the calculations. A set of nonlinear parameters \(a_n, b_k\) for simplicity was chosen in the form \(a_n = a_0 \alpha^n, b_k = b_0 \beta^k\) and the variation of parameters \(a_0, \alpha, b_0, \beta\) was used to minimize energy values. As it is usual for the variational method, the precision falls down with increasing the excitation number \(N\). To reach more precise energy values, a set of trial functions was limited by the condition \(l > L - \lambda_0\) or even less restrictive condition \(l > L - \lambda_0 - 1\) instead of \(\lambda < \lambda_0\). Convergence of the calculated energies with increasing the number of trial functions was obtained and results are presented in Table 1. Some information on this calculation can be found also in [12]. Energies of the \(L, N\) states of \(^4{\text{He}}\bar{p}\) and \(L - 1, N\) states of \(^3{\text{He}}\bar{p}\) are very close to each other.

| Table 1: Calculated energies \(E_{LN}(\text{a.u.})\) for five lowest energy levels of the \(^3{\text{He}}\bar{p}\) systems in the range \(31 \leq L \leq 37\) |
|---|---|---|---|---|
| \(^4{\text{He}}\bar{p}\) | \(L\) | \(E_{L1}\) | \(E_{L2}\) | \(E_{L3}\) | \(E_{L4}\) |
| 32 | -3.3534091 | -3.2272500 | -3.1161769 | -3.0183048 |
| 33 | -3.2158963 | -3.1049859 | -3.0075402 | -2.9219136 | -2.8355338 |
| 34 | -3.0931201 | -2.9959130 | -2.9107010 | -2.8359650 | -2.7685835 |
| 35 | -2.9836255 | -2.8988545 | -2.8247010 | -2.7597140 | -2.7007897 |
| 36 | -2.8862911 | -2.8126761 | -2.7483976 | -2.6920660 | -2.6389254 |
| 37 | -2.7999636 | -2.7364076 | -2.6809542 | -2.6320110 | -2.5853018 |

| \(^3{\text{He}}\bar{p}\) | \(L\) | \(E_{L1}\) | \(E_{L2}\) | \(E_{L3}\) | \(E_{L4}\) | \(E_{L5}\) |
|---|---|---|---|---|---|
| 31 | -3.3484555 | -3.2190748 | -3.1056452 | -3.0061026 |
| 32 | -3.2073388 | -3.0940418 | -2.9949034 | -2.9082665 | -2.8309327 |
| 33 | -3.0817523 | -3.0490121 | -2.9567378 | -2.8714926 | -2.7974268 |
| 34 | -2.9702506 | -2.8844813 | -2.8097982 | -2.7270256 | -2.6539447 |
| 35 | -2.8714926 | -2.7974268 | -2.7330406 | -2.6763097 | -2.607897 |
| 36 | -2.7843183 | -2.7207232 | -2.6654633 | -2.6161392 | -2.5853018 |
By using the method of laser-induced resonant annihilation, till now, wavelengths of five transitions \(35, 4 \rightarrow 34, 4\) \([8]\), \(34, 3 \rightarrow 33, 3\) \([13]\), \(35, 2 \rightarrow 34, 4\), \(34, 3 \rightarrow 33, 5\), \(35, 3 \rightarrow 34, 3\) \([14]\) in \(^4\text{He}\)\(\bar{p}\) and two transitions \(34, 4 \rightarrow 33, 4\), \(33, 3 \rightarrow 32, 3\) \([14]\) in \(^3\text{He}\)\(\bar{p}\) were measured with high accuracy. The calculated and experimental wavelengths are in agreement with an accuracy not worse than \(5 \cdot 10^{-4}\) and more elaborate trial functions are needed to reach a higher accuracy in the energy calculation. Recently, V. I. Korobov has obtained more precise spectra and transition wavelengths of an antiprotonic helium, using the correlated trial functions in variational calculations \([15]\).

4 Radiative transitions

Due to large lifetimes of metastable states against the Auger decay and collisional de-excitation the radiative transitions become the most important to describe the evaluation of the antiprotonic helium atom. As far as only dipole transitions are significant, the total angular momentum changes by unity in each transition. Thus, the system looses the angular momentum and energy step-by-step and finally reaches the state with a large Auger decay rate.

The rate of the dipole transition \(LN \rightarrow L_1N_1\) is given by

\[
w = \frac{4}{3(2L + 1)} |\alpha(E_{LN} - E_{L_1N_1})|^3 |M_d|^2 \frac{me^4}{\hbar^3} s^{-1},
\]

where \(\alpha = e^2 / \hbar c\) is the fine structure constant and the reduced matrix element of the dipole transition is defined in the form

\[
M_d = \langle \Psi_{L_1N_1} | |r + \rho| |\Psi_{LN}\rangle.
\]

Variational wave functions \(\Psi_{LN}\) and energies \(E_{LN}\) have been obtained as described in the previous section and used in (4), (5) to calculate the radiative transition rates. These results are presented in Table 2. A convergence of the calculated values with increasing the number of trial functions provides an estimate of the relative accuracy on the level of one per cent. The radiative transition rates calculated in papers \([10\), [16\), [17\] are fairly close to each other and to present results. The important feature is the predominance of transitions between states of the same \(N\), i. e. the approximate conservation of the excitation number in the radiative transitions. Thus, radiative cascades in an antiprotonic helium proceed almost independently along the chains of states of fixed \(N\). However, for higher excitation numbers the probabilities of interchain transitions become more significant and such transitions will be taken into account for the cascade description.

As in the energy calculation, there is a correspondence of the \(L, N\) state of \(^4\text{He}\)\(\bar{p}\) and the \(L - 1, N\) state of \(^3\text{He}\)\(\bar{p}\) and the radiative transition rates of the corresponding states are almost the same. At the same time, the \(^3\text{He}\)\(\bar{p}\) transition rates systematically exceed those of \(^4\text{He}\)\(\bar{p}\) in accordance with the difference of experimental lifetimes of the antiprotonic helium atoms \([4\). However, the explanation of this difference is not simple because the mean lifetime depends also on another processes and a significant difference in populations of the corresponding states was found in the recent experiments for different isotopes \([14\).
Table 2: Radiative transition rates $w(10^5 \text{s}^{-1})$ from the $LN$ to $L_1N_1$ state of the $^3\text{He}^-\text{pe}$ systems. Only transition rates $w \geq 10^4 \text{s}^{-1}$ are presented.

| transition $4\text{He}^-\text{pe}$ | $w$ | transition $3\text{He}^-\text{pe}$ | $w$ |
|-----------------------------------|-----|-----------------------------------|-----|
| $37,1\rightarrow36,1$             | 6.733 | $35,5\rightarrow34,5$          | 3.143 |
| $37,2\rightarrow36,1$             | 0.159 | $34,1\rightarrow33,1$          | 7.744 |
| $37,2\rightarrow36,2$             | 5.859 | $34,2\rightarrow33,2$          | 7.554 |
| $37,3\rightarrow36,2$             | 0.441 | $34,3\rightarrow33,1$          | 0.206 |
| $37,3\rightarrow36,3$             | 4.907 | $34,3\rightarrow33,3$          | 6.926 |
| $37,4\rightarrow36,3$             | 0.742 | $34,4\rightarrow33,1$          | 0.288 |
| $37,4\rightarrow36,4$             | 3.990 | $34,4\rightarrow33,2$          | 0.137 |
| $37,5\rightarrow36,4$             | 1.218 | $34,4\rightarrow33,3$          | 0.355 |
| $37,5\rightarrow36,5$             | 2.947 | $34,4\rightarrow33,4$          | 6.073 |
| $36,1\rightarrow35,1$             | 7.249 | $34,5\rightarrow33,1$          | 0.355 |
| $36,2\rightarrow35,2$             | 6.531 | $34,5\rightarrow33,2$          | 0.365 |
| $36,3\rightarrow35,2$             | 0.333 | $34,5\rightarrow33,4$          | 0.728 |
| $36,3\rightarrow35,3$             | 5.644 | $34,5\rightarrow33,5$          | 4.840 |
| $36,4\rightarrow35,3$             | 0.637 | $33,1\rightarrow32,1$          | 7.720 |
| $36,4\rightarrow35,4$             | 4.685 | $33,2\rightarrow32,2$          | 7.859 |
| $36,5\rightarrow35,4$             | 1.077 | $33,3\rightarrow32,1$          | 0.648 |
| $36,5\rightarrow35,5$             | 3.323 | $33,3\rightarrow32,3$          | 7.492 |
| $35,1\rightarrow34,1$             | 7.629 | $33,4\rightarrow32,1$          | 1.166 |
| $35,2\rightarrow34,2$             | 7.123 | $33,4\rightarrow32,2$          | 0.570 |
| $35,3\rightarrow34,2$             | 0.205 | $33,4\rightarrow32,3$          | 0.151 |
| $35,3\rightarrow34,3$             | 6.331 | $33,4\rightarrow32,4$          | 6.798 |
| $35,4\rightarrow34,3$             | 0.137 | $33,5\rightarrow32,1$          | 3.503 |
| $35,4\rightarrow34,4$             | 0.509 | $33,5\rightarrow32,2$          | 1.537 |
| $35,5\rightarrow34,4$             | 5.327 | $33,5\rightarrow32,3$          | 0.321 |
| $35,5\rightarrow34,1$             | 0.168 | $33,5\rightarrow32,4$          | 0.434 |
| $35,5\rightarrow34,2$             | 0.187 | $33,5\rightarrow32,5$          | 0.730 |
| $35,5\rightarrow34,4$             | 1.059 | $34,5\rightarrow33,2$          | 0.244 |
Lifetimes of the \((L, N) = (35, 4)\) and \((L, N) = (34, 3)\) states of \(^4\text{He}\bar{p}\) system were determined experimentally by the method of resonant laser–induced annihilation \([9]\), \([13]\). Table 3 contains the experimental decay rates and theoretical radiative transition rates of these states. One of the most probable reasons for the difference of experimental and

| \(L, N\) | Experiment \([10]\) | \([13]\) | \([9]\) | present |
|-------|----|----|----|-------|
| 35, 4 | 0.72 ± 0.02 | 0.614 | 0.619 | 0.597 |
| 34, 3 | 1.18 ± 0.04 | 0.734 | 0.754 | 0.713 |

all the theoretical values indicates the substantial contribution of additional nonradiative decay channels. As a density dependence of the lifetime of the \((34,3)\) state in \(^4\text{He}\bar{p}\) has been found in recent experiments \([14]\), collisions with surrounding atoms contribute to the decay processes. An extrapolation of the new experimental data to zero density gives \(0.91 ± 0.15\mu\text{s}^{-1}\), which is close to the theoretical radiative transition rate. The density effect probably takes place also for the \(35,4\) state and the remaining discrepancy may be caused by an additional decay process, e. g. the Auger decay.

5 Energy–level splitting due to relativistic interactions

The precise measurement of transition energies of antiprotonic helium atoms in recent experiments on the laser-induced resonant annihilation \([8]\), \([9]\) invokes the theoretical description of energy spectra with a comparable accuracy. That description of energy spectra requires to take into account the relativistic corrections of an order of \(\alpha^2\) to the pure Coulomb interaction.

Since the contribution to energies from relativistic interactions depends on the antiproton mass, charge and magnetic moment, these calculations can be used for the precise determination of the antiproton properties. This knowledge is essential in testing the fundamental symmetry principles \([18]\).

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 \(10\text{GHz}\) and without much difficulty can be improved to \(1\text{GHz}\) \([19]\). 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 within each multiplet. Calculation of the former large splitting is discussed in this section. More details of this calculation were presented in \([20]\).

For each pair of particles \(i, j\) in the three-body system the relativistic correction of an order of \(\alpha^2\) to the pure Coulomb two-body potential can be described by the Breit interaction \(U_{ij}^{(B)}\). The correction to the kinetic energy of an order of \(\alpha^2\) for each particle
\[ \Delta T_i = -\frac{\alpha^2 p_i^4}{8 m_i^2} \]  
\[(6)\]

Full relativistic correction \( H_r \) of an order of \( \alpha^2 \) to the three-body nonrelativistic Hamiltonian is a sum of \( U_{ij}^{(B)} \) for all pairs of particles and \( \Delta T_i \) for all particles

\[ H_r = \sum_i \Delta T_i + \sum_{i>j} U_{ij}^{(B)}. \]  
\[(7)\]

In the definition of the expressions \( U_{ij}^{(B)}, \Delta T_i \) in eq. (7) it is proposed that particles momentum \( p_i \) will be taken in the center of mass system of three particles \([21]\).

The interaction \( H_r \) given in (7) conserves the sum \( J = L + \sum_i s_i \) of the total angular momentum \( L = l + \lambda \) and particle spins \( s_i \). Each level of the nonrelativistic Hamiltonian splits into four and eight sublevels for \(^4\text{He}\bar{p}e\) and \(^3\text{He}\bar{p}e\) 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 \( s_3 \). Taking into consideration only terms responsible for the splitting in (7), this part of relativistic interaction can be written as follows:

\[ H_s = \alpha^2 \left( \frac{1}{\rho^3} \lambda s_3 + \frac{1}{2|\mathbf{r} - \rho|^3} [\mathbf{r} - \rho, \mathbf{q}] s_3 - \frac{1}{m_2|\mathbf{r} - \rho|^3} [\mathbf{r} - \rho, \mathbf{p}] s_3 + \frac{2}{m_1 \rho^3} [\rho, \mathbf{p}] s_3 \right) \]  
\[(8)\]

While the last two terms in (8) are inversely proportional to the masses of heavy particle \( m_{1,2} \), their contribution to the energy splitting is nevertheless comparable to the contribution from the first two terms for 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 a nonzero splitting value from the first two terms in (8).

The interaction \( H_s \), given in (8), conserves the sum \( j = L + s_3 \) of the total angular momentum \( L \) and electron spin \( s_3 \) 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 \(^4\text{He}\bar{p}e\) and \(^3\text{He}\bar{p}e\) systems, respectively. Values of this secondary splitting are much smaller in comparison with the splitting arisen due to the interaction with the electron spin (8).

Since the splitting is small in comparison with energy differences between states of different \( L \) values, the energy shift \( \Delta j_{jLN} \) for the state with quantum numbers \( j, L, N \) can be found in the first order of perturbation theory in \( H_s \)

\[ \Delta j_{jLN} = \langle \Psi_{jLN} | H_s | \Psi_{jLN} \rangle, \]  
\[(9)\]
spin. Level splitting \( \Delta E_{LN} = \Delta_{L+1/2N} - \Delta_{L-1/2N} \) is a difference of shifts (9) for \( j = L \pm 1/2 \).

Due to smallness of the relativistic interaction, radiative transitions proceed only between states of the same \( j \). For this reason, each spectral line of the transition from the state \( L_i N_i \) to state \( L_f N_f \) is to be split into a doublet with the interline distance \( \Delta \nu = \Delta E_{L_i N_i} - \Delta E_{L_f N_f} \).

Splitting values \( \Delta E_{LN} \) for a number of states of the \(^{3,4}\text{He}\bar{p}e\) systems in the range of experimentally observed values of the total angular momentum \( L \) have been calculated as described above by using variational nonrelativistic wave functions \( \Psi_{LN} \). These values are presented in Table 4.

| \( N \) | \( L=32 \)  | \( L=33 \)  | \( L=34 \)  | \( L=35 \)  | \( L=36 \)  | \( L=37 \)  |
|-------|-------------|-------------|-------------|-------------|-------------|-------------|
| 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       |             |             |

### Table 4: Splitting values \( \Delta E_{LN} \) \((10^{-6}\text{au})\) of the lowest levels in the \(^{3,4}\text{He}\bar{p}e\) systems.

| \( N \) | \( L=31 \)  | \( L=32 \)  | \( L=33 \)  | \( L=34 \)  | \( L=35 \)  | \( L=36 \)  |
|-------|-------------|-------------|-------------|-------------|-------------|-------------|
| 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 (8), the form of the wave function at small interparticle distances is the most important in evaluating the integral (9). Convergence of the calculated splitting values \( \Delta E_{LN} \) provides a few per cent relative accuracy. It is worthwhile to mention that due to a better description of the small \( N \) states in the variational method, the accuracy of calculation for the \( L, N \) state increases with decreasing \( N \). At the same time an accuracy of calculation decreases with decreasing \( L \) due to decreasing the multipolarity \( \lambda_0 \) of the Auger decay for large \( L \). Moreover, it is impossible to trace the convergence in the case of short-lived states due to a small multipolarity \( \lambda_0 < 3 \) 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 states with large enough \( N \), especially, in the \(^{3}\text{He}\bar{p}e\) system. These are the reasons to omit the above-mentioned cases in Table 4.

The last two terms in eq. (8) 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 a better understanding of the splitting dependence on \( L, N \), this contribution is presented in Table 5 for the \(^{4}\text{He}\bar{p}e\) system. The contribution to the energy–level splitting from the first two terms in (8) is of opposite sign and smaller in
magnitude. Nevertheless, this contribution decreases with increasing $L$ and compensates the $L$ dependence of the last two terms in eq. (8) providing a very slow dependence of the total splitting $\Delta E_{LN}$ on $L$. Due to almost exact conservation of the $j$ value in the radiative transition the spectral line splitting will be found as a difference of $\Delta E_{LN}$ presented in Table 4. Most appropriate for the experimental measurement are the favoured transitions between states of the same $N$, which have the largest radiative rates \cite{12,17,10}. 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 nearest future \cite{19} is aimed at searching for the splitting in unfavoured transitions $(L, N) \rightarrow (L - 1, N + 2)$.

To measure splitting in experiments on the laser-induced resonant annihilation, the initial state should be long-lived. This is provided by the condition that the multipolarity of the Auger decay for this state is $\lambda_0 = 4$. 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 $\lambda_0 = 3$. The spectral line splitting $\Delta \nu$ for a number of suitable transitions is presented in Table 6. These values are of an order of the experimentally measurable value $\sim 1$GHz. One of the recently discovered \cite{14} unfavoured transitions $(35,2 \rightarrow 34,4)$ in $^4\text{He}^\bar{\text{p}}\bar{\text{e}}$ is a good candidate for the splitting measurement.

Energy–level splitting $\Delta E_{LN}$ decreases with increasing the excitation number $N$ and an obvious reason for this dependence is decreasing of the wave function at small interparticle distances for excited states. One can mention an appreciable difference in the $\Delta E_{LN}$ dependence on $N$ for the $^4\text{He}^\bar{\text{p}}\bar{\text{e}}$ and $^3\text{He}^\bar{\text{p}}\bar{\text{e}}$ systems. As a consequence, an appreciable isotopic effect appears also for the spectral line splitting $\Delta \nu$.

### Table 5: Contribution of the last two terms in $N_s$ to the energy–level splitting $\Delta E_{LN}$ \((10^{-6}\text{au})\) in the $^4\text{He}^\bar{\text{p}}\bar{\text{e}}$ 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  |        |        |

### Table 6: Spectral line splitting $\Delta \nu = \Delta E_{LiNi} - \Delta E_{LfNf}$ (GHz) for the transitions $L_iN_i \rightarrow L_fN_f$ in the $^3,^4\text{He}^\bar{\text{p}}\bar{\text{e}}$ systems.

| $^4\text{He}^\bar{\text{p}}\bar{\text{e}}$ | $^3\text{He}^\bar{\text{p}}\bar{\text{e}}$ |
|-----|-----|
| $L_iN_i \rightarrow L_fN_f$ | $\Delta \nu$ | $L_iN_i \rightarrow L_fN_f$ | $\Delta \nu$ |
| 33,1$\rightarrow$32,3 | -0.92 | 32,1$\rightarrow$31,3 | -0.53 |
| 34,1$\rightarrow$33,3 | -0.86 | 33,1$\rightarrow$32,3 | -0.86 |
| 34,2$\rightarrow$33,4 | -0.91 | 33,2$\rightarrow$32,4 | -1.22 |
| 35,2$\rightarrow$34,4 | -0.87 | 34,2$\rightarrow$33,4 | -1.35 |
| 35,3$\rightarrow$34,5 | -0.34 |        |        |
The following considerations can be used to understand qualitatively the $L, N$–dependence of the energy–level splitting. The 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 $H_s$ (8). This contribution is proportional to the relative momentum of heavy particles $p$. One can consider that the motion of heavy particles is approximately the same as in a hydrogen–like atom and the 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 5. The contribution from the first two terms in the splitting interaction $H_s$ is connected with the electron rotation and is proportional to a small component of the wave function arising due to polarization of an electron by an antiproton. With decreasing $L$ the antiproton moves to the region of increasing electron density and the polarization increases. In this way, contributions to the energy–level splitting from the last two terms in $H_s$ and the remaining part of splitting interaction are of opposite sign and level off the dependence of the total splitting $\Delta E_{LN}$ on $L$.

One can consider quasi-classically that the antiproton orbit became more stretched with increasing $N$ at a fixed total angular momentum. For this reason all the terms of the splitting interaction $H_s$ decrease with increasing $L$ and provide the $N$ dependence presented in Tables 4, 6.

6 Auger decay

In addition to the radiative transitions, the important decay channel of antiprotonic helium atoms is the emission of an electron with the $^3, ^4He\bar{p}$ hydrogen-like ion formation, i.e. the Auger decay. The main feature of the Auger decay rates of antiprotonic helium atoms is the essential dependence on the transition multipolarity, i.e. the smallest angular momentum of the outgoing electron $\lambda_0$. As discussed in Section 2, calculated eigenenergies $E_{LN}$ [10], [17], [12] unambiguously determine the transition multipolarities $\lambda_0$ by the condition $\varepsilon_{L-\lambda_0} < E_{LN}$.

Apart from the early calculation of Russell [6] the only progress in the calculation of the Auger decay rates is due to the paper [16]. It was found that the Auger decay rate decreases about three orders of magnitude with increasing the smallest angular momentum of the outgoing electron $\lambda_0$ by one.

As the Auger lifetime of states with $\lambda_0 = 3$ and $\lambda_0 = 4$ is of an order of $10^{-8}$ s and $10^{-5}$ s, respectively, and the radiative lifetime is about $10^{-6}$ s [10], [17], [12], the resonant laser-induced transitions between states of $\lambda_0 = 3$ and 4 became observable in the experiments [8], [9]. For this reason, the most important thing is to calculate the Auger decay rates for the states of $^3, ^4He\bar{pe}$ systems with multipolarities $\lambda_0 = 3, 4$. The method and results of the calculation are presented in [22] and will be described in this section. One should mention that there are no other calculations of the Auger decay rate for the $^3He\bar{pe}$ system and the presented results allow one to consider the isotopic effect in this process.

The Auger decay rates of the antiprotonic helium atom are very small in the atomic scale and the very fine details of the discrete state wave functions $\Psi_{LN}$ and continuum wave functions $\Psi_c$ will be accurately determined. In particular, since $\Psi_{LN}$ and $\Psi_c$ belong to the
closed- and open-channel subspaces, respectively, the orthogonality condition $\langle \Psi_{LN} | \Psi_c \rangle = 0$ will be strictly fulfilled. As described in Section 2, $\Psi_{LN}$ is an eigenfunction of the approximate Hamiltonian $H_{LN}$ and projector $P_{LN}$. As a consequence, $\Psi_c$ should be an eigenfunction of the projector $1 - P_{LN}$ and can be found as a solution of the equation

$$(1 - P_{LN})H(1 - P_{LN})\Psi_c = E_{LN}\Psi_c. \quad (10)$$

Thus, the orthogonality requirement is fulfilled and the perturbation theory can be applied due to smallness of the decay rates.

According to the Feshbach orthogonal projection method the decay rate $\Lambda$ is

$$\Lambda = \frac{1}{\sqrt{2\mu_3(E - \varepsilon_l)}}|M_{tr}|^2 \frac{m_3 e^4}{\hbar^2} s^{-1}, \quad (11)$$

where $1/\mu_3 = 1/(m_1 + m_2) + 1/m_3$ and the transition matrix element is

$$M_{tr} = \langle \Psi_c | (1 - P_{LN})H P_{LN} | \Psi_{LN} \rangle. \quad (12)$$

Since the continuum wave function is naturally described in the Jacobi coordinates $\mathbf{r}, \mathbf{\rho}_1$, these coordinates will be used in this calculation.

The contribution to $M_{tr}$ is negligible for the $\Psi_c$ components, corresponding to $(l, \lambda_1)$ eigenvalues of angular momenta $l, \lambda_1$ if $l \neq l_0, \lambda_1 \neq \lambda_0$. For this reason, only the $(l_0, \lambda_0)$ component will be taken into account in the calculation of $\Psi_c$.

Due to the large centrifugal barrier the continuum wave function $\Psi_c$ can be taken as a product of the normalized wave function of $^{3,4}\text{He}^-\mathbf{p}$ and the function $f(\mathbf{\rho}_1)$ describing the relative motion of an electron and $^{3,4}\text{He}^-\mathbf{p}$. As the total angular momentum of the system is $L$ and its projection is $M$, $\Psi_c$ takes the form

$$\Psi_c(\mathbf{r}, \mathbf{\rho}_1) = A Y_{l_0\lambda_0}^L(\hat{\mathbf{r}}, \hat{\mathbf{\rho}}_1) r^{l_0} e^{-ar} f(\mathbf{\rho}_1) = \Phi(\mathbf{r}, \mathbf{\rho}_1) f(\mathbf{\rho}_1). \quad (13)$$

In the framework of this approach the interaction of the outgoing electron and the remaining $^{3,4}\text{He}^-\mathbf{p}$ ion is described by the folding potential

$$V_0(\mathbf{\rho}_1) = \langle \Phi | (1 - P_{LN})H(1 - P_{LN}) | \Phi \rangle, \quad (14)$$

and the radial function $f(\mathbf{\rho}_1)$ obeys the ordinary differential equation.

Due to the large centrifugal barrier for the outgoing electron, the Auger decay rate is mainly determined by the wave functions in the large $\mathbf{\rho}_1$ range, where the interaction of the electron and $^{3,4}\text{He}^-\mathbf{p}$ system is nearly a sum of the Coulomb and centrifugal potential. Indeed, the replacement of the folding potential by the Coulomb one gives rise to a minor change in the matrix element. This fact supports the applicability of the approximation (13).

500–650 trial functions $\chi_{n\kappa\lambda_1}^{LM}(\mathbf{r}, \mathbf{\rho}_1)$ (3) of the variables $\mathbf{r}, \mathbf{\rho}_1$ have been used in the variational calculation of $\Psi_{LN}, E_{LN}$. As described above, to fulfill the strict requirement of orthogonality, only trial functions satisfying the condition $l > l_0$ have been taken into account. The largest contributions to the transition matrix element $M_{tr}$ come from the $(l, L - l)$ components of the wave function and they have been treated with special
care. An additional set of 70–130 trial functions with specific nonlinear parameters have been used to describe these components. As the calculated energy values are in good agreement with the results of [12], one can conclude that the present calculations provide the accurate description of antiprotonic helium atoms. Using $\Psi_{LN}, E_{LN}$ and $\Psi_c(r)$ in the form (13) the Auger decay rates $\Lambda$ have been calculated according to equations (11), (12). These results are presented and compared with [16] in Table 7. To understand the role of the wave function structure in this calculation, the largest contributions of the $(l, \lambda_1)$ components of $\Psi_{LN}$ to the transition matrix element are presented in Table 8. It is worthwhile to mention that the exponentially small part of the wave function in the large $\rho_1$ region is important in evaluating the integral (12). As it follows from the numerical results, the essential point in the calculation of the Auger decay rates is to determine very fine features of the wave function. Really, the largest contribution to the transition matrix element comes from the smallest component corresponding to the largest possible $\lambda_1$ value (Table 8) and contributions to the $M_{tr}$ from the $(l, \lambda_1)$ components of $\Psi_{LN}$ compensate each other due to alternation of signs. Moreover, the most important in the calculation of $M_{tr}$ is the large $\rho_1$ region of the configuration space, where these components decrease exponentially.

As a result, uncertainty in the calculated decay rates for the multipolarity $\lambda_0 = 3$ is of an order of 10 per cent. As is indicated in Table 7, the decay rates for the $^4\text{He}\bar{\text{p}}\bar{\text{e}}$ system in this case are in agreement with the results of [16]. The calculated decay rate of the (34,4) state of this system is in fairly good agreement with experimental lifetime $\tau =$

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Table 7: Multipolarities $\lambda_0$ and Auger decay rates $\Lambda \ (s^{-1})$ of $^{3,4}\text{He}\bar{\text{p}}\bar{\text{e}}$

| $^{4}\text{He}\bar{\text{p}}\bar{\text{e}}$ | $^{3}\text{He}\bar{\text{p}}\bar{\text{e}}$ |
|---|---|
| L,N | $\lambda_0$ | $\Lambda$ | $\Lambda [10]$ | L,N | $\lambda_0$ | $\Lambda$ |
| 34,4 | 3 | $7 \cdot 10^7$ | $8.5 \cdot 10^7$ | 33,4 | 3 | $2 \cdot 10^8$ |
| 33,3 | 3 | $1.2 \cdot 10^8$ | $1.5 \cdot 10^7$ | 32,3 | 3 | $3.4 \cdot 10^8$ |
| 32,2 | 3 | $1.1 \cdot 10^8$ | $4.0 \cdot 10^7$ | 31,2 | 3 | $3.3 \cdot 10^8$ |
| 35,4 | 4 | $\sim 5 \cdot 10^4$ | $6.7 \cdot 10^2$ | 34,4 | 4 | $\sim 10^4$ |
| 34,3 | 4 | $\sim 1 \cdot 10^5$ | $2.7 \cdot 10^4$ | 33,3 | 4 | $\sim 10^4$ |

*K. Ohtsuki, private communication

Table 8: Normalized contributions to the transition matrix element $M_{tr}(l, \lambda_1)$ from the $(l, \lambda_1)$ components of the wave function for two states of the $^4\text{He}\bar{\text{p}}\bar{\text{e}}$ system.

| $(L,N)=(34,3)$ $\lambda_0=4$ | $(L,N)=(34,4)$ $\lambda_0=3$ |
|---|---|
| $(l, \lambda_1)$ | $M_{tr}(l, \lambda_1)$ | $(l, \lambda_1)$ | $M_{tr}(l, \lambda_1)$ |
| 34,0 | -0.28 | 34,0 | 0.24 |
| 33,1 | 0.51 | 33,1 | -0.46 |
| 32,2 | -0.38 | 32,2 | 1.22 |
| 31,3 | 1.14 |
15ns \[8\]. At the same time, for the (33,3) state the calculated decay rate twice exceeds the experimental value \(\tau=16.6\text{ns}\) \[13\].

On the contrary, the case of the transition multipolarity \(\lambda_0 = 4\) is rather complicated for calculation due to much smaller values of the transition matrix element, and only an estimate of the decay rate can be obtained. These values exceed significantly the results obtained in \[16\].

The calculated decay rates of the \(^3\text{He}\bar{\text{p}}\) system reveal the substantial isotopic dependence. In fact, decay rates of the (33,4) and (32,3) states of \(^3\text{He}\bar{\text{p}}\) are about three times as large as those of analogous (34,4) and (33,3) states of \(^4\text{He}\bar{\text{p}}\). At the same time, other characteristics of the \((L - 1, N)\) state of \(^3\text{He}\bar{\text{p}}\) are close enough in comparison with the \((L, N)\) state of \(^4\text{He}\bar{\text{p}}\). As for \(\lambda_0 = 4\) transitions of \(^3\text{He}\bar{\text{p}}\), in this case the calculated decay rates can be estimated only to an order of magnitude and isotope effect is uncertain.

Thus, the Auger decay rates have been calculated for the multipolarities \(\lambda_0 = 3, 4\). The method of calculation should be improved to determine with more precision the small components of the wave function and small decay rates in the cases of higher multipolarities \(\lambda_0 \geq 4\). Isotopic effect has been found and the role of the structure of the wave function has been studied. The Auger decay rates of metastable states \(\lambda_0 = 3\) amount to tenth of the radiative transition rates and can be important in cascade processes. If the isotopic effect for the \(\lambda_0 = 3\) states is the same as for \(\lambda_0 = 4\) states, the Auger decay in \(^3\text{He}\bar{\text{p}}\) can compete with radiative transitions.

### 7 Conclusions

Properties of new three-body systems, the recently discovered antiprotonic helium atoms and analogous hadron–containing systems are intensively investigated both theoretically and experimentally. The investigation of intrinsic properties of antiprotonic helium atoms, their formation and collisions with atoms and molecules is necessary for understanding the antiproton fate in media. The coexistence of a particle and an antiparticle in the same atomic system brings on the principal possibility to study antiproton properties by precise measurements of antiprotonic helium atoms.

Nonstability and an extremely large total angular momentum \(L \sim 30 - 40\) of these exotic systems give rise to significant difficulties in the theoretical treatment of this system. However, due to very long lifetimes the metastable states of these systems are treated as true bound states and the variational approach is applied in the calculation. Variational eigenfunctions and eigenenergies are used to obtain the radiative transition rates, energy-level splitting due to relativistic interactions and Auger decay rates of antiprotonic helium atoms. The radiative transitions and Auger decay determine the cascade process after the formation of antiprotonic helium. Calculation of the energy-level splitting will be helpful in the proposed measurement of the multiplet structure \[19\]. One can mention that these rather different values are sensitive to different parts of the wave function, e. g. the region of small interparticle distances is important in the calculation of energy-level splitting and the asymptotic region is important in the calculation of Auger decay rates.

A simple set of trial functions used in the calculations, nevertheless, provides a description of rather different properties of antiprotonic helium atoms. Convergence of the
calculated values with increasing the number of trial functions has been achieved and the isotopic effects have been investigated by comparison of the calculated properties of $^4\text{He}\bar{p}$ and $^3\text{He}\bar{p}$. In this respect, one should mention the investigation of $^6\text{He}\bar{p}$ having in mind that the reduced-mass ratio for $^6\text{He}\bar{p}$ and $^4\text{He}\bar{p}$ is almost the same as for $^4\text{He}\bar{p}$ and $^3\text{He}\bar{p}$.

The calculated wave functions can be used also to consider more complicated problems; the most important of them is the determination of formation probabilities and initial populations. Due to substantial density and impurity effects found in experiments [4], [14], [23], other important applications are the interaction of antiprotonic helium atoms with usual helium atoms and diatomic molecules. As for the Auger decay, more efforts are needed to calculate small components of the wave function in the asymptotic region in cases of higher multipolarities $\lambda_0 \geq 4$.

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References

[1] Yamazaki T. e.a., Phys. Rev. Lett., 1989, vol. 63, p. 1590
[2] Nakamura S. N. e.a., Phys. Rev. A, 1992, vol. 45, p. 6202
[3] Iwasaki M. e.a., Phys. Rev. Lett., 1991, vol. 67, p. 1246
[4] Nakamura S. N. e.a., Phys. Rev. A, 1994, vol. 49, p. 4457
[5] Condo G. T., Phys. Lett., 1964, vol. 9, p. 65
[6] Russell J. E., Phys. Rev. A, 1970, vol. 1, p. 721; p. 735; p. 742
[7] Ahlrichs R., Dumbrajs O., Pilkuhn H. and Schlaile H. G., Z. Phys. A, 1982, vol. 306, p. 297
[8] Morita N. e.a., Phys. Rev. Lett., 1994, vol. 72, p. 1180
[9] Hayano R. S. e.a., Phys. Rev. Lett., 1994, vol. 73, p. 1485 (1994); vol. 73, p. 3181
[10] Shimamura I., Phys. Rev. A, 1992, vol. 46, p. 3776
[11] Kartavtsev O. I., Few–Body Systems Suppl., 1995, vol. 8, p. 228
[12] Kartavtsev O. I., Proc. of the 3rd Intern. Symp. on Muon and Pion Interactions with Media, Dubna, 1995, p. 138
[13] Maas F. e.a., Phys. Rev. A, 1995, vol. 52, p. 4266
[14] Widmann E. e. a., 1995, Proc. of the Third Conference on Nucleon–Antinucleon Physics, Moscow, Yad. Fiz., (in print)
[15] Korobov V. I., Proc. of the Intern. Symp. on Muon Catalyzed Fusion, Dubna, 1995, Hyperfine Interactions (in print)

[16] Morita N., Ohtsuki K. and Yamazaki T., Nucl. Instr. Meth. A, 1993, vol. 330, p. 439

[17] Yamazaki T. and Ohtsuki K., Phys. Rev. A, 1992, vol. 45, p. 7782

[18] Charlton M., Eades J., Horvath D., Hughes R. O., Zimmermann C., Phys. Rep. 1994, vol. 241, p. 65

[19] PS205 Collaboration, 1995, Preprint CERN SPSLC 95–12/SPSLC I 201

[20] Kartavtsev O. I., Proc. of the International Symposium on Exotic Atoms and Nuclei, Hakone, Japan, 1995, Hyperfine Interactions (in print)

[21] Lev F. M., Riv. Nuova Cim. 1993, vol. 16, p. 1

[22] Fedotov S. I., Kartavtsev O. I., Monakhov D. E., 1995, Proc. of the Third Conference on Nucleon–Antinucleon Physics, Moscow, Yad. Fiz. (in print); JINR Rapid Communications, 1995, No. 5 (73), p. 13

[23] Widmann E. e. a., Phys. Rev. A, 1995, vol. 51, p. 2870