Collisions of cold antiprotonic helium atoms and ions with ordinary helium atoms

G Ya Korenman and S N Yudin
Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, 119991 Moscow, Russia
E-mail: korenman@nucl-th.sinp.msu.ru

Abstract. We consider two types of collisional processes with excited antiprotonic helium systems. (i) Transitions between hyperfine structure sublevels in $(\bar{p}\text{He}^+)_n_{LJ}$ are considered at $T \leq 25$ K using the coupled-channels method and a model of scalar and tensor interactions between antiprotonic and ordinary He atoms. Inelastic cross sections for the single and double spin-flip transitions are less than elastic ones by four and seven orders of magnitude, respectively. The cross sections show a resonance behaviour at $E \sim 1 - 4$ K, and therefore the relaxation rates, density shift and broadening of the M1 spectral lines decrease with increasing temperature from 3 to 25 K. (ii) Stark transitions and induced annihilation during collisions of the $(\bar{p}\text{He}^{2+})_{nl}$ ion with He atoms at $E \sim 10$ K are considered for all $l$-states at $n \sim 30$ in the framework of the coupled-channels method. In order to take into account complex energy shifts of the $ns$ and $np$-states, we introduce modified boundary conditions in these channels. The main contribution to elastic scattering, Stark transitions and induced annihilations during collisions comes from the long-range polarization interaction. Admixtures of $ns$ and $np$-states to $nl$-states ($l \geq 2$) during collisions induce the effective annihilation cross sections for the initial $l$ up to 15, but don’t affect the Stark cross sections for states with nearly-circular orbits. The calculated values for both types of processes are compatible with recent experimental data.

1. Introduction
The experimental discovery and investigation of the metastable antiprotonic states in helium have opened a new chapter in the study of antiprotonic atoms (see a comprehensive review [1] of the results obtained up until 2001). In addition to the fundamental properties of the antiproton, these investigations give interesting insights into the interaction of antiprotonic helium with ordinary atoms and molecules. These data stimulated many theoretical papers on the mechanisms of antiprotonic helium formation, on collisional quenching of the metastable states, on effects of collisional (density) shift and broadening of E1-spectral lines, etc. Further study of antiprotonic helium by the ASACUSA collaboration at CERN will bring new data that pose specific problems in the theory of collisional effects at low temperature ($\sim 10$ K). For the measurements of hyperfine splittings of antiprotonic helium levels by a triple laser-microwave-laser resonance method [2], it is important to estimate the rates of collisional transitions between the HFS sublevels, and the density shifts and broadenings of the microwave M1 spectral lines. The first observation of cold long-lived antiprotonic helium ions ($\bar{p}\text{He}^{2+}$) with lifetimes $\tau_i \sim 100$ ns against annihilation [3] revealed an unexpected $n$-dependence and isotope effect for effective annihilation rates in circular states ($l = n-1$) at $n = 28-32$. Earlier considerations of collisional processes of ($\bar{p}\text{He}^{2+}$) at higher energy could not explain these data.
In this paper we consider two types of processes: (i) collisional transitions between the HFS sublevels in neutral antiprotonic helium

\[(\bar{p}\text{He}^+)_{nLFJ} + \text{He} \rightarrow (\bar{p}\text{He}^+)_{nLF'J'} + \text{He}, \tag{1}\]

and (ii) Stark transitions and induced annihilations in the antiprotonic helium ion

\[(\bar{p}\text{He}^{+2})_{nl} + \text{He} \rightarrow \begin{cases} (\bar{p}\text{He}^{+2})_{nl'} + \text{He} & \text{(Stark)}, \\ (\pi \ldots \pi X) + \text{He} & \text{(annihilation)}. \end{cases} \tag{2}\]

For both types of collisions we use the quantum close-coupling method with the appropriate interatomic interactions. In the case of the antiprotonic ion, a modification of the boundary conditions at \(R \rightarrow \infty\) in the channels corresponding to \(ns\) and \(np\)-states is introduced in order to take into account the annihilation widths of the states.

2. Collisional effects on HFS transitions in antiprotonic helium atoms

Hyperfine splitting of the \(nl\)-states of antiprotonic helium arise due to magnetic interaction between the orbital angular momentum \(L\) and the spins of the electron and of the antiproton \([1, 4]\). We denote the HFS states with definite \(F = L \pm s_e\) and \(J = F \pm s_p\) in order of energy: \(|1\rangle = |F = L + 1/2, J = L\rangle, |2\rangle = |F = L + 1/2, J = L + 1\rangle, |3\rangle = |F = L - 1/2, J = L - 1\rangle\) and \(|4\rangle = |F = L - 1/2, J = L\rangle\).

Data on the hyperfine structure of the \((n, L) = (37, 35)\) state of \((\bar{p}\text{He}^+)\) were obtained by a triple laser-microwave-laser resonance method \([2]\). The central frequencies of microwave M1-transitions, \(\nu_{HF}^+(4 \rightarrow 2) = 12.89596(34)\) GHz and \(\nu_{HF}^+(3 \rightarrow 1) = 12.92467(29)\) GHz, are in excellent agreement \((\lesssim 30\) ppm) with calculations \([4]\) for the isolated \((\bar{p}\text{He}^+)\) system. The results suppose that the density shift of the M1 spectral lines is a very small, less than the experimental accuracy \((\sim 300\) kHz), in contrast with the \(E1\) transitions \([1]\). The width of the lines \((\gamma \sim 5.3 \pm 0.7\) MHz) leaves room for a collisional broadening. The data suggest also that the mean time of the collisional relaxation \(\tau_c\) exceeds the observation time window \((140\) ns).

In order to estimate the collisional characteristics, we introduce a model \([5]\) of scalar and tensor interactions between the excited antiprotonic helium and an ordinary atom,

\[\langle nLA|V(R, \xi)|nLA'\rangle = V_0(R)\delta_{AA'} + V_2(R)\sum_{\nu} \langle L\Lambda'2\nu|L\Lambda\rangle Y_{\nu}^*(n)\sqrt{4\pi/\delta}, \tag{3}\]

where \(V_0(R) = -C_6 f(R), V_2(R) = -C_6 f(R) g(R), f(R) = (R^2 - r_c^2)/(R^2 + r_0^2)^2\). The scalar term has a repulsion at \(R < r_c\), a Van der Waals minimum at \(R_0^2 = (r_0^2 + 4r_c^2)/3\) and the long-range asymptote of \(-C_6/R^6\). The factor \(g(R) = 1 - \exp(-\eta R^2)\) with \(\eta \sim 10\) a.u. tends to 1 at \(R \gtrsim 1\) a.u. and ensures a correct dependence \((\sim R^2)\) of the tensor term at \(R \rightarrow 0\). In the calculations we use two sets of parameters: \((A) C_6 = 2.82, r_c = 3.0, r_0 = 2.8\) a.u. from the fitting \([6]\) of the density shifts of \(E1\)-transitions; \((B) C_6 = 3.35, r_c = 4.75, r_0 = 0.707\) a.u., estimated from the data \([7, 8]\) of ab initio calculations of the potential energy surface. For both sets we adopt \(C_6 = -0.37C_6^0\) from the independent-particle model of \((\bar{p}\text{He}^+)\) with effective charges. The tensor term in \((3)\) couples states with different \(F, J\). Due to the small kinetic energy \((E \lesssim 25\) K), the basis is restricted to the 4 HFS states at fixed \(nL\) and to relative angular momenta up to \(L_R = 5\). We solve coupled-channels equations within this basis, obtain the \(S\)-matrix and calculate elastic and inelastic (spin-flip) cross sections and the rates of the transitions between HFS states averaged over the thermal velocity distribution. Typical results for elastic and inelastic (spin-flip) cross sections are shown in Fig. 1. All cross sections have a maximum at \(E_m \simeq 4\) K for parameter set \(A\). For parameter set \(B, E_m < 1\) K. The results show
Figure 1. Cross sections of $(pHe^+)_{nL} - He$ collisions vs. c.m. kinetic energy: (a) elastic cross section $\sigma_{44}$ for the state $|4\rangle$; (b) electron spin-flip cross section $\sigma_{42}$; (c) double spin-flip cross section $\sigma_{41}$. Solid and dashed lines refer to parameter sets A and B.

that the collisional transitions can be classified by a spin-flip similarity. The cross sections of single electron spin-flip transitions ($\Delta F = \Delta J = \pm 1$) or single antiproton spin-flip transitions ($\Delta F = 0, \Delta J = \pm 1$) are very close within the relevant pairs, e.g., $\sigma(4 \rightarrow 2) \approx \sigma(3 \rightarrow 1)$, $\sigma(4 \rightarrow 3) \approx \sigma(2 \rightarrow 1)$. The cross sections of all single spin-flip transitions are of the same order of magnitude, $\sigma(4 \rightarrow 2) \sim \sigma(4 \rightarrow 3)$, etc., and less than elastic cross sections by four orders of magnitude. The cross sections of the double spin-flip transitions ($\Delta F = \pm 1, \Delta J = 0, \pm 2$) are smaller by three orders of magnitude than single spin-flip cross sections. The same relationships remain valid for the transition rates $\lambda(i \rightarrow j) = N\langle \sigma_{ij}v \rangle$. Due to averaging over thermal motion, these values decrease with temperature for $E_{\text{th}} < T < 25$ K (see Fig. 2a). At higher temperatures the rates could increase due to contributions of higher partial waves.

Figure 2. Temperature dependencies of per-atom values: (a) collisional transition rate $\lambda(4 \rightarrow 2)/N$, (b) density shift $\Delta/N$ of the M1 spectral line $4 \rightarrow 2$, (c) density broadening $\gamma/N$ of the same line. Solid and dashed lines refer to parameter sets A and B.

Density shifts $\Delta$ and broadenings $\gamma$ of the microwave M1 transitions ($FJ \rightarrow F'J'$) are also expressed in terms of the S-matrix at the binary collision conditions [9]. We calculate the
complex value $\gamma + i\Delta$ using Eq. (57.96) for non-overlapping levels from [9]. The results for the spectral line $4 \rightarrow 2$ are shown in Figs. 2b and 2c.

In the triple-resonance experiment [2], collisional transitions ($i \neq j$) can change the relative populations of the upper (4, 3) and lower (2, 1) groups of the levels during the time between the two laser pulses. At $T = 6 K$, $N = 3 \times 10^{20}$ cm$^{-3}$ we obtain $1/\lambda(4 \rightarrow 2) = 160$ and 325 ns for $A$ and $B$, respectively. Both values are compatible with the experimental limit of the relaxation time $\tau_d > 140$ ns. At the same $T$ and $N$ we have found the density shift of M1 spectral lines for the favored transitions ($\Delta F = \pm 1, \Delta J = \pm 1$): $\Delta\nu \simeq 80$ and 87 kHz with the sets $A$ and $B$, respectively. This value is less than experimental accuracy ($\simeq 300$ kHz) of the measured values $\nu_{HF}$, and therefore the density shift could not be revealed in the experiment [2]. The calculated broadening of the same spectral lines is $\gamma = 5.9$ and 2.7 MHz for $A$ and $B$, respectively. These values are also compatible with the experimental width (5.3 $\pm$ 0.7 MHz) of the observed M1 spectral lines.

3. Stark transitions and induced annihilation in antiprotonic helium ions

In order to consider the processes (2) we introduce the interaction between a ($\bar{p}$He$^{+2}$)$_{ml}$ ion and an ordinary He atom in the form

$$V(R, r) = V_0(R) + (d \cdot \nabla R) V_0(R) + (Q_2(r) \cdot C_2(R)) V''(R),$$

where $V_0(R)$ is adiabatic potential of the interaction between the He atom and the charge (+1) of the ion, and $d$ and $Q_{2\mu}$ are dipole and quadrupole operators that can mix $nl$ states of the ion. The potential $V_0(R)$ is approximated [10] by a sum $V_0(R) = V_3(R) + V_p(R)$ of a Morse potential $V_3(R) = D_0 \{\exp[-2\beta(R - R_c)] - 2 \exp[-\beta(R - R_c)]\}$ and of a long-range polarization interaction cut off at an intermediate distance, $V_p(R) = -\alpha \cdot g_p(R)/(2R^2)$, where $g_p(R) = [1 - \exp (-\gamma(R - R_c)^2)]$ at $R > R_c$, and $g_p(R) = 0$ at $R < R_c$. The adopted values of the parameters are [10, 11] $D_0 = 0.075$, $R_c = 1.46$, $\beta = 1.65$, $\alpha = 1.383$, $\gamma = 0.005$ a.u.

Antiprotonic helium ions in states with $l \geq 2$ can be considered to be hydrogen-like systems with the nuclear charge $Z = 2$ and reduced mass $\mu \simeq 1467 m_e$ for $^4$He and $1376 m_e$ for $^3$He. However ns and np-states have complex energy shifts $\Delta E_{nl} = -\epsilon_{nl} - i\Gamma_{nl}/2$ due to strong nuclear interactions and annihilations of the antiproton. Dependence of $\Delta E_{nl}$ on $n$ is well known from the theory, $\Delta E_{ns} = \Delta E_{ls}/n^4$, $\Delta E_{np} = 32(n^5 - 1)/(3n^3) \cdot \Delta E_{2p}$. The remaining parameters are taken from the experimental data and theoretical calculations using optical model. For $^4$He we take $\Gamma_{ls} = 11$ keV, $\Gamma_{2p} = 36$ eV, $\epsilon_{nl} = 0.3\Gamma_{nl}$.

Traditional close-coupling methods suppose an expansion of the total wave function in terms of inner stationary states of colliding subsystems. In the case of the ($\bar{p}$He$^{+2}$)$_{ml}$ ion, a similar expansion has to involve, inter alia, ns and np-states with large annihilation widths. The life times $\tau_{nl} = h/\Gamma_{nl}$ are small as compared with the collision time and mean time between subsequent collisions, and therefore these states cannot be presented in the incoming channels and, moreover, the corresponding components of the wave function of relative motion in outgoing channels have to damp out at large distances. For a correct consideration of the close-coupling equations involving the annihilating states we divide the total space of $N$ channels into the subspace $\alpha$ of the stationary states and the subspace $\beta$ of the annihilating states. Then we construct two types of $(N \times N)$ matrix solutions $X(R)$ and $Y(R)$, which are defined by the asymptotic forms at $R \rightarrow \infty$: $X_{ij}, Y_{ij} \rightarrow 0$ at $i \neq j$ in the both subspaces, $X_{ii}$ and $Y_{ii}$ at $i \in \alpha$ tend to ordinary incoming and outgoing waves, respectively, whereas at $i \in \beta X_{ii} \equiv 0$, $Y_{ii}$ tend to damping outgoing waves with complex wave number $k_\beta (1m_k \beta > 0)$. The total matrix of solutions with the correct asymptotic behaviour $F(R) = X(R) - Y(R)C$ has to be sew at a small $r = r_s$ with the $(N \times N)$ matrix of regular solutions obtained by a standard way taking into account the complex energy shifts in the annihilating channels. This procedure yields the submatrix $C_{\alpha\alpha} = S$, which is the S-matrix of the transitions between the states in the subspace $\alpha$. 

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α. The S-matrix is not unitary, because the hamiltonian of the problem is non-hermitian. The unitary defect $(1 - \sum_{j \in \alpha} |S_{ji}|^2)$ gives the cross section of induced annihilation for the initial state $i \in \alpha$.

With interaction (4) and complex shifts of $ns$ and $np$-states we have solved the coupled-channel equations using the basis that includes all states with different $l$ at fixed $n$ and relative angular momenta up to $L_R = 12$ at $E \sim 10$ K. Cross sections of elastic scattering, of partial $\sigma(nl \rightarrow nl'; E)$ and total $\sigma_{Sl}(nl; E)$ Stark transitions and of induced annihilation $\sigma_a(nl; E)$ at initial $l \geq 2$ were obtained. The relative importance of different terms in the interaction can be illustrated by the total cross sections of the Stark transitions from the circular state with $n = 30$ at $E = 10$ K. If we take into account in (4) the short-range Morse potential for $V_0(R)$ and the dipole term, the cross section is about 120 a.u. When the polarization term $V_p(R)$ is added to $V_0(R)$, the same cross section rises to 620 a.u., but the addition of the quadruple term changes the cross section by the negligible value (< 0.2%). Therefore the main part of the calculation was done without the quadruple interaction.

Figure 3 shows the dependence of total Stark and of induced annihilation cross sections on initial $l$ ($n = 30$, $E = 10$ K). The curve 1 is obtained without including the annihilation width.

Figure 4 shows the energy dependence of the total Stark cross sections for circular orbits with $n = 30$ for $^4$He (full curve) and $^3$He (dashed curve).
Per-atom rates of Stark transitions from circular orbits, \( \kappa_{St} = \langle v_{\sigma St} \rangle \), averaged over thermal motion at \( T = 10 \) K, are given in Table 1 for the two isotopes. The calculated values cannot be compared directly with the experimental values \([3]\) of per-atom effective annihilation rates \( d\gamma/d\rho \sim (1 - 3) \cdot 10^{-16} \text{ MHz } \cdot \text{cm}^3 \), because the latter rates are a result of many cascade processes. Nevertheless, Stark transitions from circular orbits can be considered as the most important first step of the cascade, because they change the inner angular momentum of the antiprotonic ion and open up possibilities for other processes. It is important that the values of \( \kappa_{St} \) are greater than (but of the same order of value as) the experimental rates \( d\gamma/d\rho \). Moreover, we obtain also that \( \kappa_{St} \) for \(^3\)He is greater than for \(^4\)He and grows with \( n \), and these are correlated with the observed dependencies of the value \( d\gamma/d\rho \).

Table 1. Per-atom Stark transition rates at \( T = 10 \) K for circular orbits of the two helium isotopes (units \( 10^{-16} \text{ MHz } \cdot \text{cm}^3 \)).

| isotope | \( n = 28 \) | \( n = 30 \) | \( n = 32 \) |
|---------|--------------|--------------|--------------|
| \(^4\)He | 3.77         | 4.15         | 4.46         |
| \(^3\)He | 4.46         | 4.82         | 5.01         |

4. Conclusion

We have considered two types of collisional processes with excited antiprotonic helium systems at very low energy: (i) transitions between hyperfine structure sublevels in \((\bar{p}\text{He}^+)_{nLFJ}\) and (ii) Stark transitions and induced annihilation during collisions of \((\bar{p}\text{He}^{2+})_{nl}\) ions with He atoms, using a coupled-channels method and rather simple models of interaction between the antiprotonic helium atom or ion and an ordinary atom. We give also a generalization of the close-coupling method with annihilating states included in the basis. The results for the processes under consideration are compatible with recent experimental data.

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