объединенный
институт
ядерных
исследований
дубна

E4-93-151

V.I.Korobov, Yu.A.Kuperin*, S.I.Vinitsky

ANTIPROTONIC MOLECULES — A NEW EXOTIC THREE-BODY SYSTEM

Submitted to «Physics Letters B» and International Conference «NAN-93», Moscow, September, 1993

---

*Department of Mathematical & Computational Physics, Institute for Physics, St.Petersburg University, St.Petersburg, Russia

1993

Introduction

Exotic three-body Coulomb systems drew attention of many authors for a long period of time. The existence of the positronium negative ion, $Ps^- = e^-e^-e^+$, has been predicted many years ago [1], while it was detected experimentally rather recently [2]. Now this system is well studied and the contemporary variational calculation gives both exact binding energy value and the annihilation lifetime of 0.47936ns [3] which is in a good agreement with the experimental data 0.478 ± 0.02ns [4].

The existence of a bound state for the protonium positive ion, $Pr^+ = pp\bar{p}$, consisting of two protons (in the singlet spin state) and a negatively charged antiproton is evident. It can be easily obtained by the simple mass scale transformation from the Ps^- ion.

At the same time it will be interesting to investigate the existence of other antiproton ions with hydrogen isotopes p, d and t. The study of these systems has definite interest because there are exist two competitive processes like an annihilation and a nuclear fusion that gives an opportunity to investigate nuclear interactions at the low energy region.

This work treats a three particle system as a purely Coulombic. We presume that the nuclear forces can be taken into account as a perturbative correction. This assertion seems reasonable because the protonium atom ($Pr = p\bar{p}$) radius $a_{p\bar{p}} = 57.6$fm significantly exceeds the characteristic nuclear size $r_0 = 1.7$fm which defines the effective radius of nuclear short-range potential [5].

Basic results

After separating of the center-of-mass motion, the nonrelativistic Hamiltonian of a three-particle system can be written in units $\hbar = e = m_e = 1$ as

$$H = -\frac{1}{2\mu_a}\Delta_{\mathbf{r}_a} - \frac{1}{2\mu_b}\Delta_{\mathbf{r}_b} - \frac{1}{m_{\bar{p}}}\nabla_{\mathbf{r}_a}\nabla_{\mathbf{r}_b} - \frac{1}{r_a} - \frac{1}{r_b} + \frac{1}{r_{ab}} \qquad (1)$$

where r_a and r_b are the vectors from an antiproton to nuclei a and b, respectively, r_{ab} is the vector connecting nuclei a and b, $\mu_i = m_{\bar{p}}m_i/(m_{\bar{p}} + m_i)$ are the reduced masses of the corresponding antiprotonic atoms.

As a trial function we shall use the explicitly-correlated Slater-type basis of functions, which has a good convergence for this kind of problems [6, 7, 8]. Since our investigation concerns with only S-state molecular systems we shall write out the wavefunction in a form

$$\Psi(\mathbf{r}_a,\mathbf{r}_b) = \sum_{i=1}^{K} C_i e^{-\alpha_i r_a - \beta_i r_b - \gamma_i r_{ab}}, \quad \text{for heteronuclear states}$$
$$\Psi(\mathbf{r}_a,\mathbf{r}_b) = (1-P_{ab}) \sum_{i=1}^{K} C_i e^{-\alpha_i r_a - \beta_i r_b - \gamma_i r_{ab}}, \quad \text{for homonuclear states} \tag{2}$$

where P_{ab} is the permutation operator of particles a and b. Nonlinear exponents are generated according to the formulas

$$\begin{aligned} \alpha_i &= A\langle \tfrac{1}{2}k(k+1)\sqrt{2}\rangle, \\ \beta_i &= B\langle \tfrac{1}{2}k(k+1)\sqrt{3}\rangle, \\ \gamma_i &= C\langle \tfrac{1}{2}k(k+1)\sqrt{5}\rangle - \min(\alpha_i,\beta_i), \end{aligned} \tag{3}$$

where $\langle x\rangle$ is the fractional part of x. Quantities A, B, C are variational parameters of the trial function.

We have also investigate the possible existence of P-states for considered exotic molecules. But our very careful calculations have shown that it is conceivable that there are no such states.

Our numerical results are collected in Table 2 as well as mean distances between particles in a molecule expressed in units $m_{\bar{p}} = 1$. The masses used were $m_p = m_{\bar{p}} = 1836.1515 m_e$, $m_d = 3670.481 m_e$, $m_t = 5496.918 m_e$ and the Rydberg energy was $R_\infty = 13.6058041$eV. For the convenience of comparison Table 1 contains the necessary characteristics of corresponding antiprotonic atoms.

The scope of our interests is to estimate the nuclear fusion and annihilation rates from the molecular states. To do that we make use the so-called G-factor and γ-factors which can be determined like δ-function operators at different coalescence points:

$$\begin{aligned} G &= |F(0)|^2 = \int |\Psi(r_a,r_b,r_{ab})|^2_{r_{ab}=0}\, d\tau, \\ \gamma^m_{n\bar{p}} &= \int |\Psi(r_a,r_b,r_{ab})|^2_{r_n=0}\, d\tau, \qquad n = a,b. \end{aligned} \tag{4}$$

The calculated values of these quantities are presented in Table 3. The expression for the fusion rate has been given by Jackson[9] as

$$\lambda_f = A_s|F(0)|^2 = \frac{S(0)|F(0)|^2}{(1+\delta_{ab})\pi c \alpha m}, \tag{5}$$

where α is the fine structure constant, c is the velocity of light, $m = m_a m_b/(m_a+m_b)$ is the reduced mass of the nuclei and $S(E)$ is the fusion charge-independent cross section factor. The nuclear reactions which can be observed

Table 1: Binding energies, $E_{a\bar{p}}$(eV), reduced masses, $\mu_{a\bar{p}} = (m_a^{-1} + m_{\bar{p}}^{-1})^{-1}$, γ-factors, $\gamma^a_{a\bar{p}} = (\pi a^3_{a\bar{p}})^{-1}$, $a_{a\bar{p}} = a_e/\mu_{a\bar{p}}$, mean sizes, $< r >_{a\bar{p}}$, and mean-square sizes, $< r^2 >_{a\bar{p}}$, of the hydrogen isotope atoms in the ground state (in units $m_{\bar{p}} = 1$).

	$p\bar{p}$	$d\bar{p}$	$t\bar{p}$
$E_{a\bar{p}}$(eV)	12491.16	16652.12	18726.91
$\mu_{a\bar{p}}$	0.5	0.6666	0.7496
$\gamma^a_{a\bar{p}}$	3.979(-2)	9.427(-2)	1.341(-1)
$< r >_{a\bar{p}}$	3	2.250	2.001
$< r^2 >_{a\bar{p}}$	12	6.752	5.339

Table 2: Binding energies, ϵ(eV), mean sizes, $< r_{ab} >$, $< r >_{a\bar{p}}$, $< r >_{b\bar{p}}$, and mean-square sizes, $< r^2_{ab} >$, $< r^2 >_{a\bar{p}}$, $< r^2 >_{b\bar{p}}$, of antiprotonic molecular ions (in units $m_{\bar{p}} = 1$). $M_a \geq M_b$.

	$pp\bar{p}$	$dd\bar{p}$	$tt\bar{p}$	$dt\bar{p}$
ϵ(eV)	599.829	966.691	1260.787	319.151
$< r_{ab} >$	8.55	5.80	4.80	6.51
$< r >_{a\bar{p}}$	5.49	3.85	3.26	2.54
$< r >_{b\bar{p}}$	5.49	3.85	3.26	5.79
$< r^2_{ab} >$	93.1	41.5	27.7	56.6
$< r^2 >_{a\bar{p}}$	48.4	22.6	15.6	9.37
$< r^2 >_{b\bar{p}}$	48.4	22.6	15.6	51.4

Table 3: The square of the wave function amplitude (Eq.(4)) at coalescent points, G, γ^m_a, γ^m_b, (in units $m_{\bar{p}} = 1$), $M_a \geq M_b$. Fusion rates, λ_f, from the antiprotonic molecular states (in s^{-1}).

	$pp\bar{p}$	$dd\bar{p}$	$tt\bar{p}$	$dt\bar{p}$
G	1.712(-4)	2.579(-4)	2.381(-4)	1.974(-4)
γ^m_a	2.073(-2)	5.011(-2)	7.242(-2)	1.036(-1)
γ^m_b	2.073(-2)	5.011(-2)	7.242(-2)	2.650(-2)
$\frac{\gamma^m_{a\bar{p}}}{\gamma^a_{a\bar{p}}} + \frac{\gamma^m_{b\bar{p}}}{\gamma^a_{b\bar{p}}}$	1.042	1.063	1.080	1.053
λ_f	3.4(-9)	8.1(14)	7.4(14)	1.1(17)

from experiments are

$$
\begin{aligned}
p+p &\xrightarrow{A_s=4.7^{-40}} d+e^{+}+\overline{\nu}+2.2\text{MeV}, \\
d+d &\xrightarrow{A_s=7.5^{-17}} \begin{cases} {}^{3}He+n+3.3\text{MeV}, \\ t+p+4.0\text{MeV}, \end{cases} \qquad (6)\\
d+t &\xrightarrow{A_s=1.3^{-14}} {}^{4}He+n+17.6\text{MeV}, \\
t+t &\xrightarrow{A_s=7.5^{-17}} {}^{4}He+2n+11.3\text{MeV},
\end{aligned}
$$

where the fusion constant A_s is expressed in cm^3s^{-1}. The nuclear fusion constants were evaluated from the values of $S(0)$ tabulated by Fowler, Caughlan and Zimmerman [10], these numbers have uncertainties of up to 200%. Table 3 shows the calculated fusion rates from the considered molecular states.

To estimate the branching ratio of two possible channels of an ion decay we can use the experimental data of annihilation width of $1S$ state of $p\bar{p}$ atom $\Gamma_{1S} \approx 1\text{keV}$ and that this width has a few isotope dependence [11]. The nuclear shift to the energy level of the ground state is equal to $\text{Re}(\Delta E_{1S}) \approx 0.7\text{keV}$ [12].

Annihilation rates from the molecular state can be calculated as a ratio of gamma-factors of a molecular state and a corresponding $\bar{p}$-atom $1S$ state

$$\lambda^{m}_{ann} = \left\{ \frac{\gamma^{m}_{a\bar{p}}}{\gamma^{a}_{a\bar{p}}} + \frac{\gamma^{m}_{b\bar{p}}}{\gamma^{a}_{b\bar{p}}} \right\} \lambda^{a}_{ann}, \qquad (7)$$

where $\lambda^{a}_{ann} = \Gamma/\hbar \approx 1.5 \cdot 10^{18}\text{s}^{-1}$ is the annihilation rate of an $\bar{p}$-atom. We have estimated the values of the multiplicative factor in (7) (see Table 3) and obtained that this factor insignificantly deviates from the unity. That lead us to the conclusion that the annihilation rates from these molecular states are approximately the same as from the ground state of the $p\bar{p}$ atom.

Recently, there was published a work [13] presenting an estimation of annihilation/fusion ratio of about 10^3 for the $dt\bar{p}$ bound state that differs from our results by two orders of magnitude due to the very rough estimation given in [13].

Conclusions

As it is known, the concept of an antimatter and speculations on its existence have more than nine decades history [14]. The discovery of the metastable states of the helium "atomcules" $\bar{p}He^{+}$ [15]

$$\bar{p} + He \longrightarrow \bar{p}He^{+} + e, \qquad (8)$$

shows the possible way for the antihydrogen $\bar{H}$ production, see, for example, [16]:

$$Ps + \bar{p}He^{+} \longrightarrow \bar{H} + He, \qquad (9)$$

and renews an interest to the atom-antiatom rearrangement collisions [17]

$$\bar{H} + H \longrightarrow Pr + Ps. \qquad (10)$$

If we substitute the hydrogen gas by the DT mixture we probably can observe the reaction of the $dt\bar{p}$ molecular ion formation:

$$\bar{H} + DT \longrightarrow [dt\bar{p}e] + Ps. \qquad (11)$$

The other, probably, more realistic way to observe this state is the direct collision of $\bar{p}$ with DT molecules. Stopping by the DT molecule the antiproton replaces one electron on its orbit occupying the level with principal quantum number (n) close to

$$n_0 = (M^{*}/m_e)^{1/2} \approx 35,$$

where M^{*} is the reduced mass of $\bar{p}$ with respect to the nucleus (d or t). A hydrogen-like atom in this state has a strong attractive potential $\sim \alpha/R^2$ in the field of a charged particle due to the linear Stark effect and series of three-body resonances below its thresholds. It makes possible the following cascade reaction:

$$\bar{p} + DT \longrightarrow [dt\bar{p}e]^{*} + e^{-} \longrightarrow (dt\bar{p})^{+} + 2e^{-}, \qquad (12)$$

where $[dt\bar{p}e]^{*}$ is some resonant state. For a muon stopping in DT mixture the discussion of the similar processes can be found in [18].

It shoud be noted that the fusion reaction of the nuclei d and t in the $dt\bar{p}$ ion takes place at the energy greater than that of the corresponding $dt\mu$ ion. Therefore one can anticipate an essential increasing of the fusion rate for the d and t nuclei in the $dt\bar{p}$ ion in comparision with the corresponding rate for the $dt\mu$ ion. Thus the ratio of the fusion and annihilation rates could be essential greater than the values indicated in the present work. This effect is now in progress and in the case of it being considerable one can discuss the antiproton catalyzed fusion.

References

[1] J.A. Wheeler, Ann. N. Y. Acad. Sci., **48**, (1946) 219.

[2] A.P. Mills, Jr., Phys. Rev. Lett., **46**, (1981) 717.

[3] A.K. Bhatia, R.J. Drachman, Phys. Rev. A, **28**, (1981) 2523; Y.K. Ho, J. Phys. B, **16**, (1983) 1503.

[4] A.P. Mills, Jr., Phys. Rev. Lett., **50** (1983) 671.

[5] V.S. Popov, Preprint ITEP 87-136, Moscow, Atominform, 1987.

[6] A.J. Thakkar and V.H. Smith Jr., Phys. Rev. A, **15**, (1987) 1.

[7] A.M. Frolov and V.D. Efros, J. Phys. B, **18**, (1985) L265.

[8] S.A. Alexander and H.J. Monkhorst, Phys. Rev. A, **38**, (1988) 26.

[9] J.D. Jackson, Phys. Rev., **106** (1957) 330.

[10] W.A. Fowler, G.R. Caughlan and B.A. Zimmerman, Ann. Rev. Astron. Astrophys., **5** (1967) 525.

[11] G. Reifenröther and E. Klempt, Phys. Lett. B, **245** (1990) 129; S. Wycech, A.M. Green and J.A. Niskanen, Phys. Lett. B, **152** (1985) 308.

[12] B.O. Kerbikov, L.A. Kondratyuk and M.G. Sapozhnikov, Usp. Fiz. Nauk, **159** (1989) 1.

[13] A.M. Frolov and A.J. Thakkar, Phys. Rev. A, **46** (1992) 4418.

[14] A. Schuster, Nature (Lond.) **58** (1898) 367; 618.

[15] T. Yamazaki, Nucl. Phys. A, **543** (1992) 229.

[16] T. Yamazaki, Z. Phys. A, **341** (1992) 223.

[17] D.L. Morgan. Jr. and V.W. Hughes, Phys. Rev. A, **7** (1973) 1811.

[18] G.Ja. Korenman, V.P. Popov and G.A. Fesenko, Muon Catalyzed Fusion, **7** (1992) 179.

Received by Publishing Department
on April 30, 1993.