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LOW ENERGY INELASTIC COLLISIONS OF EXCITED HYDROGEN MESIC ATOMS

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The advanced adiabatic approach previously proposed for the description of the collisional problems in atomic physics is extended to the specific case of mesic atom collisions in the excited states $n \geq 2$. The calculations of muon transfer and Coulomb deexcitations rates at the collisions of $(p\mu)_n$, $(d\mu)_n$ and $(t\mu)_n$ muonic atoms in excited states $n = 3, 4, 5$ with hydrogen isotopes p, d, t are presented.

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1. There are several problems in muonic physics, weak interaction physics and especially in physics of muon catalyzed fusion (see e.g. [1]) which need the cross-sections of different collisional processes of hydrogen isotope mesic atoms in the excited states $n \leq 6$ at collision energy $0.001 \leq \varepsilon \leq 100$ eV, $(a, b) = (p, d, t)$, particularly:

muon transfer:

$$(b\mu)_n + a \xrightarrow{\lambda_n} (a\mu)_n + b\,; \tag{1}$$

Coulomb deexcitation:

$$(a\mu)_n + b \xrightarrow{\lambda_{nn'}} (a\mu)_{n'} + b\,; \qquad n' < n\,. \tag{2}$$

The main and only difference of processes (1) – (2) from the analogous atomic processes is the muon mass $m_\mu = 206.769\ m_e$, which leeds, nevertheless, to the essential modification of the code based on the advanced adiabatic approach (AAA) which was previously proposed [2–4] for the description of the analogous collisional processes in atomic physics.

In the collision energy range E $\lesssim$ 100 eV processes (1) – (2) are deep adiabatic ($v/\alpha c \lesssim 0.1$) and the relative motion of nuclei takes place in the almost static potential formed by the averaged muon and electron motion. In contrast to the atomic collisions, where the classical description of the nuclei motion is well justified, low energy mesic atomic collisions (1) – (2) at $n \geq 2$ should be considered semiclassically.

In what follows we will present the self-consistent method of the calculation of the rates of processes (1) and (2) taking into account their peculiarities mentioned. It is based on the advanced adiabatic approach [2–4, 5, 6] modified to the specific case of mesic atom collisions. The first applications of this method were presented in papers [7, 8] where the rates λ_n of the muon transfer (1) and the rates $\lambda_{nn'}$ of the Coulomb deexcitation in $(p\pi)_n$-atoms

$$(p\pi)_n + p \;\rightarrow\; (p\pi)_{n'} + p \tag{3}$$

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were calculated.

2. The Hamiltonian $\hat{H}$ of the Coulomb three-body problem (two nuclei + a muon) in Jacobi coordinates $(\mathbf{R}, \mathbf{r})$ has the form

$$\hat{H} = -\frac{1}{2M}\Delta_{\mathbf{R}} - \frac{1}{2m}\Delta_{\mathbf{r}} - \frac{Z_a}{r_a} - \frac{Z_b}{r_b} + \frac{Z_a Z_b}{R} . \tag{4}$$

Here: $\mathbf{R}$ - is the vector of the internuclear distance, $\mathbf{r}$ - is the muon coordinate, $M = (1/M_a + 1/M_b)^{-1}$ is the reduced mass of two nuclei ($M_a \geq M_b$), Z_a and Z_b are the charges of nuclei, $Z_\mu = -1$ is the muon charge, $m = (1 + 1/(M_a + M_b))^{-1}$ is the reduced mass of muon moving around nuclei and mesic atomic units are used (m.a.u., $\hbar = e = m_\mu = 1$).

The wave functions $\Psi(\mathbf{r}, \mathbf{R})$ describing reactions (1) – (2) can be decomposed over the solutions $\varphi_j(\mathbf{r}; R)$ of the Coulomb two-center problem [9]

$$\Psi(\mathbf{r}, \mathbf{R}) = \sum_j \varphi_j(\mathbf{r}; R) \frac{1}{R} F_j^J(R) Y_J(\Theta, \Phi) . \tag{5}$$

Here: J is the total angular momentum of the three-body problem, $\varphi_j(\mathbf{r}; R)$ is the complete set of the solutions of the Coulomb two center problem

$$\hat{h}\varphi_j(\mathbf{r}; R) = E_j(R)\varphi_j(\mathbf{r}; R) , \quad \hat{h} = -\frac{1}{2m}\Delta_{\mathbf{r}} - \frac{Z_a}{r_a} - \frac{Z_b}{r_b}, \tag{6}$$

describing the muon motion at fixed nuclei separated at the distance R; $j = [nn_1n_2mp]$ is the set of parabolic quantum numbers specifying the quantum state of the muon motion; (p is the state parity: g – gerade, u – ungerade), $E_j(R)$ is the energy of muon in the state j as a function of R.

After averaging over the muon motion the nuclear motion is described by the set of equations:

$$\frac{1}{2M}\frac{d^2F_i^J(R)}{dR^2} + \left[\varepsilon - U_i(R) - \frac{J(J+1)}{2MR^2}\right] F_i^J(R) = \frac{1}{2M}\sum_j U_{ij}(R) F_j^J(R) , \tag{7}$$

where $U_{ij}(R)$ are the nonadiabatic coupling potentials [9], ε is the collision energy in the entrance channel and $U_i(R)$ is the effective potential including term $E_i(R)$, the Coulomb repulsion of nuclei and taking into account the electron screening effects at $R \gg 1$ [10].

In the limit $R \to \infty$ the adiabatic terms $E_i(R)$ converge to the energies of the isolated atoms $(\mu a)_i$ and $(\mu b)_i$ with the relative accuracy $\sim M^{-1}$ only. To incorporate isotopic effects, which play the important role in processes (1) – (2), the standard adiabatic approach should be modified, using the additional transformation suggested by Solov'ev[11]. It improves the accuracy of $E_i(\infty)$ up to level $\sim M^{-2}$ and splits the degenerated pair $E_{ig}(R)$ and $E_{iu}(R)$ into pair $E_{ia}(R)$ and $E_{ib}(R)$ which represent atoms $(a\mu)_n$ and $(b\mu)_n$ correspondingly at $R \to \infty$ (see Fig.1).

3. In the leading order solutions $F_i^J(R)$ of equation (7) can be presented in the semiclassical form

$$F_i^J(R) = C_i \, [p_i^J(R)]^{-1/2} \, \exp\left\{ i \int_{c_{ij}} p_i^J(R) \, dR \right\}, \tag{8}$$

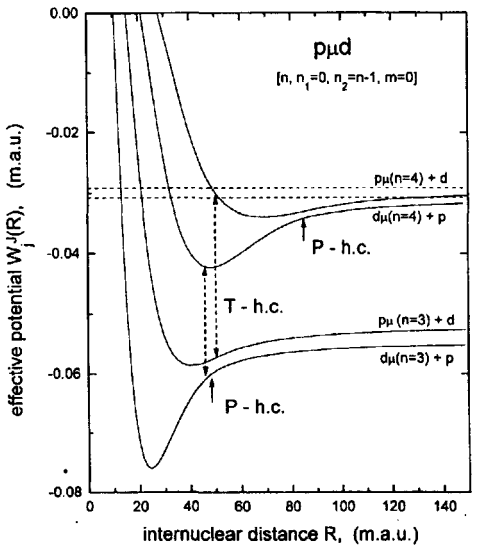

Fig.1. The scheme of transitions $i = [nn_1n_2m] \to j = [n'n'_1n'_2m]$ in the system $pd\mu$ via P and T hidden crossings for the reaction (2) of the Coulomb deexcitation

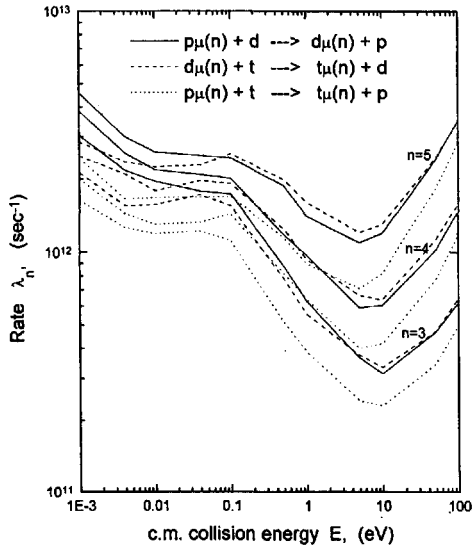

Fig.2. The rates of the muon transfer (1) $(b\mu)_n + a \to (a\mu)_n + b$ from the states $n = 3, 4, 5$

$$p_i^J(R) = \left[2M\left(\varepsilon - U_i(R) - \frac{J(J+1)}{2MR^2}\right)\right]^{1/2}.$$

According to AAA, the nonadiabatic transitions from the adiabatic state i to the state j are determined by the hidden crossings of terms $E_i(R)$ and $E_j(R)$ in the complex plane R at $R = R_c = Re\ R_c + iIm\ R_c$ where $E_i(R_c) = E_j(R_c)$.

The cross sections of the transitions $i \to j$ are calculated with the formulae [2–4]:

$$\sigma_{ij}(\varepsilon) = \frac{\pi}{p_i^2} \sum_{J=0} (2J+1) \mid S_{ji}^J \mid^2,$$

$$|S_{ji}|^2 = 2P_{ij}(1 - P_{ij}), \quad P_{ij} = e^{-2\Delta_{ij}}. \tag{9}$$

$$\Delta_{ij} = \mid \mathrm{Im} \int_{c_{ij}} p(R)dR \mid = \mid \mathrm{Im} \int_{\mathrm{Re}R_c}^{R_c} [p_i(R) - p_j(R)]\, dR \mid,$$

c_{ij} is the contour in the complex R-plane in the domain $(0, \infty)$ including the branch-point R_c.

There are four types of the hidden crossings: S-, T-, P- and Q-series [2–4]. For processes (1)–(2) only P and T series are essential. T-series connects the states $i = [nn_1n_2mp]$ and $j = [n'n'_1n'_2mp]$ with $n'_1 = n_1$, $n'_2 = n_2 + 1$ and the same parity p at $Z_a = Z_b$. P-series connects states $E_{ja}(R)$ and $E_{jb}(R)$ with the same set of the parabolic quantum numbers $[nn_1n_2m]$ at slightly different charges Z_a and Z_b. The lower term $E_{ja}(R)$ belongs to the heavier atom $(a\mu)$ and corresponds at $M_a = M_b$ to the symmetric g-state ($l = 2n_2$) and the upper term $E_{jb}(R)$ correspondes to u-state ($l = 2n_2 + 1$).

4. The numerical code for the calculation of the cross-sections of processes (1) – (2) is based on automated program-package ARSENY [5, 6]. It includes the subprograms of the calculation of terms $E_j(R)$ for states $j = [n\ n_1\ n_2\ m\ p]$, $n \leq 5$ (220 adiabatic states), search for all branch points $R_c = \mathrm{Re}R_c + i\mathrm{Im}R_c$ of the hidden crossings in the complex plane R connecting pairwise terms $E_i(R_c)$ and $E_j(R_c)$, calculation of the Stueckelberg parameters $\Delta_{ij}(R_c)$, S^J_{ji}-matrix elements, cross sections $\sigma_{ij}(\varepsilon)$, as well as the averaged cross sections $\sigma_{nn'}(\varepsilon)$ [2)]

$$\sigma_{nn'}(\varepsilon) = \sum_{n_1,n_2,n_1',n_2',m} \frac{2-\delta_{om}}{n^2}\sigma_{ij}(\varepsilon) \tag{10}$$

and transition rates

$$\lambda_{nn'} = \sigma_{nn'}\ v\ \rho_0, \tag{11}$$

where v is the relative velocity and $\rho_0 = 4.25\ 10^{22}\mathrm{cm}^{-3} = 0.73 \cdot 10^{-3}$m.a.u. is the liquid hydrogen density.

In Fig.1, where only terms $E_i(R)$ for $pd\mu$ system with $m = 0$, $\Delta = -(n-1)$ at $n = 4$ and $n = 3$ are plotted as an example, the hidden crossings (h.c.) of P- and T-types are marked by arrows. The muon transfer reaction (1) $(p\mu)_n \to (d\mu)_n$ is ruled by P-type series, only T-type series are responsible for the Coulomb deexcitation (2)

$$(d\mu)_n + p \to (d\mu)_{n-1} + p\,, \tag{12}$$

the combination of the P- and T-types is essential for the reactions

$$(p\mu)_n + d \to (p\mu)_{n-1} + d\,. \tag{13}$$

Relations (9) – (11) give the complete algorithm for the calculation of all cross sections $\sigma_{ij}(\varepsilon)$ and $\sigma_{nn'}(\varepsilon)$ at given collision energy ε.

5. The calculated rates of processes (1) – (2) are presented in Figs.2 – 4. We do not compare our results with the results of numerous publications [12 – 17] (and many others) because all of them contain a principal mistake[3)] which origin is in the following. For the description of mesic atomic collisions they all use the version of AAA developed by Solov'ev and co-workers for atomic collisions. In atomic case the typical collision energy ($\sim$ 10 keV/nucl) is much higher than potential energy of terms ($\sim$ 1 eV) and expressions (8,9) for $p_i(R)$ and Δ_{ij} can be simplified using a small parameter $2U_i(R)/Mv^2(R) \sim U_i(R)/\varepsilon \sim 10^{-4}$ in the following way:

$$p_i^J(R) = \left[2M\left(\varepsilon - U_i(R) - \frac{J(J+1)}{2MR^2}\right)\right]^{1/2} =$$

$$= \left[M^2v^2(R) - 2MU_i(R)\right]^{1/2} \approx Mv(R) - U_i(R)/v(R)$$

where

[2)] The numerical results presented in paper [8] are calculated with this formula. Eq.(9) in paper [8] contains a misprint (factor 1/2).

[3)] The comparison which was done in our previous paper [8] has shown disagreement of results [17] by an order of magnitude at low collision energies.

$$v(R) = \left[\frac{2}{M}\left(\varepsilon - \frac{J(J+1)}{2MR^2}\right)\right]^{1/2}.$$

Hence,

$$\Delta_{ij} = |\mathrm{Im}\int_{\mathrm{Re}\ R_c}^{R_c} \frac{U_i(R) - U_j(R)}{v(R)} dR| \tag{14}$$

In mesic atomic physics the typical collision energies $\varepsilon \lesssim 1\,\mathrm{eV}$, $U_i(R) \sim 100$ eV, the ratio $U_i(R)/\varepsilon \geq 10^2$ is not anymore a small parameter, and relations (14) are entirely unvalid. But just these relations with the additional dubious assertion

$$v(R) = \frac{1}{2M}\left[p_i(R) + p_j(R)\right] \tag{15}$$

were used in papers [12–17] for the calculations of the cross-sections (1) and (2).

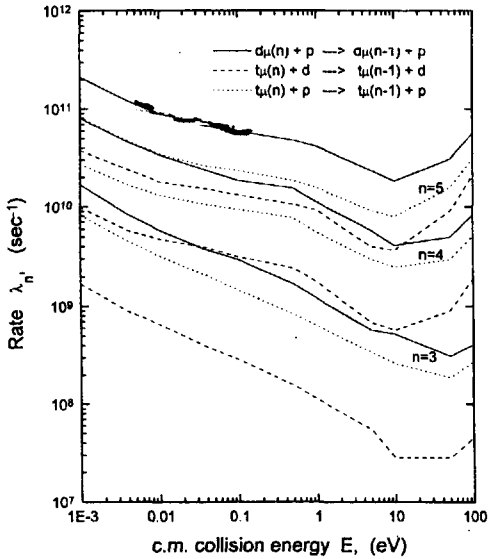

Fig.3. The rates of the Coulomb deexcitation $(a\mu)_n + b \to (a\mu)_{n-1} + b$ from the states $n = 3, 4, 5$

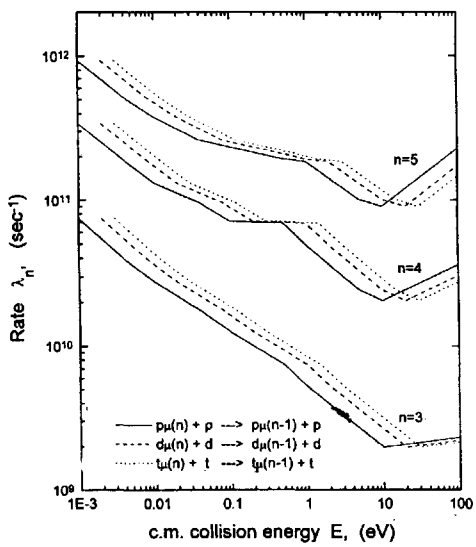

Fig.4. The rates of the Coulomb deexcitation $(a\mu)_n + a \to (a\mu)_{n-1} + a$ from the states $n = 3, 4, 5$ in symmetrical systems

6. The method presented in this paper is illustrated with the processes of muonic physics but after simple scaling the obtained results describe also the collision processes involving $a\pi^-$-, aK^-- and $a\bar{p}$-hydrogen isotope exotic atoms ($a = p, d, t$) . The rates of the Coulomb deexcitation (2) $\lambda_{nn'}$ of muonic atoms are calculated selfconsistently for the first time in this paper. This opens the way for the *ab initio* theoretical description of the kinetics cascade of exotic atoms in the hydrogen isotope mixtures.

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