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Coulomb deexcitation of muonic hydrogen within quantum close-coupling method

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The Coulomb deexcitation of muonic hydrogen in collisions with hydrogen atom has been studied in the framework of the fully quantum-mechanical close-coupling method for the first time. The calculations of the l-averaged cross sections of the Coulomb deexcitation are performed for $(\mu p)_n$ and $(\mu d)_n$ atoms in the initial states with the principal quantum number $n = 3 \div 9$ and at the relative energies $E = 0.1 \div 100$ eV. The obtained results for the n and E dependences of the Coulomb deexcitation cross sections drastically differ from the semiclassical results. Important contribution of the transitions with $\Delta n > 1$ to the total Coulomb deexcitation cross sections (up to $\sim 37\%$) is predicted.

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Introduction. Exotic hydrogen atoms are formed in the highly excited states. The ensuing deexcitation proceeds via many intermediate states up to nuclear absorption or transition to the ground state. The collisional processes play an important role in this cascade. In particular, the elastic scattering and Stark transitions decelerate while the Coulomb deexcitation (CD) accelerates the exotic atoms, influencing their quantum numbers and energy distributions. The CD process has attracted a lot of attention, especially after the "hot" πp atoms with the kinetic energy up to 200 eV were found experimentally [1, 2]. The most plausible explanation of the high energy components of the exotic atoms is that the part of the transitions from the states with $n \geq 3$ proceeds via the CD.

The theoretical study of the CD process was fulfilled up to now within three different approaches. The first results were obtained by Bracci and Fiorentini [3] in the two-state semiclassical approach with some additional approximations (hereafter referred to as BF model). Later, the CD cross sections were calculated within the advanced adiabatic (AA) approach [4, 5] (see also references therein) based on the adiabatic hidden crossing theory [6], and within the classical-trajectory Monte Carlo (CTMC) method [7]. While the CTMC and BF results are in fair agreement, the more elaborated AA approach [4, 5] gives much smaller cross sections than [3]. On the other hand, the BF and CTMC approaches cannot be expected to give the reliable results for the CD process in low-n states. Therefore, the situation in the most interesting region ($n = 3 \div 7$) is rather ambiguous and it is necessary to study the CD process within the more realistic quantum-mechanical approach.

In this paper we study the Coulomb deexcitation of $(\mu p)_n$ and $(\mu d)_n$ atoms in collisions with H, using the close-coupling method. To illustrate some gross features of the calculated cross sections we present here only the l-averaged CD cross sections.

Formalism. The close-coupling (CC) method gives a unified quantum-mechanical treatment of non-reactive scattering processes

$$(a\mu^-)_{nl} + (be)_{1s} \to (a\mu^-)_{n'l'} + (be)_{1s} \qquad (1)$$

including elastic scattering ($n' = n, l' = l$), Stark transitions ($n' = n, l' \neq l$) and Coulomb deexcitation ($n' < n$). Here a and b are nuclei of hydrogen isotopes (p, d, or t). In the present consideration, as well as in the previous studies [3, 7], we restrict ourselves to the "frozen" electron approximation, i.e. the electron state is fixed in its ground state during the collision. The CC approach can be extended in a straightforward manner to include the target electron excitations.

Total non-relativistic Hamiltonian of the four particles $(a\mu^- + be)$ in the c.m. system is given by

$$H = -\frac{1}{2m}\Delta_{\mathbf{R}} + h_\mu(\boldsymbol{\rho}) + h_e(\mathbf{r}) + V(\mathbf{r}, \boldsymbol{\rho}, \mathbf{R}). \qquad (2)$$

Here m and $\mathbf{R} = \mathbf{R}_{be} - \mathbf{R}_{a\mu}$ are the reduced mass and relative coordinate of the colliding subsystems, $\mathbf{R}_{be}$ and $\mathbf{R}_{a\mu}$ are the coordinates of the centers of mass of the atoms, $\boldsymbol{\rho} = \mathbf{r}_\mu - \mathbf{r}_a$, $\mathbf{r} = \mathbf{r}_e - \mathbf{r}_b$ are their inner coordinates. The eigenvalues and eigenfunctions of the inner Hamiltonians h_μ and h_e of the $(a\mu)$ and (be) atoms will be denoted as ε_n, $\Phi_{nlm}(\boldsymbol{\rho})$ and ϵ_{1s}, $\varphi_{1s}(\mathbf{r})$, respectively. The interaction potential

$$V(\mathbf{r}, \boldsymbol{\rho}, \mathbf{R}) = V_{ab} + V_{\mu b} + V_{ae} + V_{\mu e}, \qquad (3)$$

includes the pair Coulomb interactions $V_{\alpha\beta}$ between the particles from two colliding subsystems. The atomic units ($\hbar = e = m_e m_b/(m_e + m_b) = 1$) will be used throughout the paper unless otherwise stated.

In the framework of the method, the total wave function of the system with the definite energy E and quantum numbers of the total angular momentum J, M is presented as

$$\Psi_E^{JM}(\mathbf{r}, \boldsymbol{\rho}, \mathbf{R}) = R^{-1} \sum_{nlL} G_{nlL}^J(R) |1s, nl, L : JM\rangle, \quad (4)$$

where the basis states $|1s, nl, L : JM\rangle$ are the tensor product of inner atomic wave functions $|1s\rangle$, $|nlm\rangle$ and the relative angular momentum function $Y_{L\Lambda}(\hat{\mathbf{R}})$. The radial functions of the relative motion $G_{nlL}^J(R)$ satisfy the coupled second order differential equations

$$\left(\frac{d^2}{dR^2} + k_n^2 - \frac{L(L+1)}{R^2}\right) G_{nlL}^J(R) = \\ = 2m \sum_{n'l'L'} W_{nlL,n'l'L'}^J(R)\, G_{n'l'L'}^J(R), \quad (5)$$

where $k_n^2 = 2m(E_{cm} + \varepsilon_{n_0} - \varepsilon_n)$, E_{cm} and n_0 are the energy of the relative motion and the principal quantum number in the entrance channel. In order to obtain the matrix elements of the interaction potential (3)

$$W_{nlL,n'l'L'}(R) = \langle 1s, nl, L : JM | V | 1s, nl, L : JM\rangle \quad (6)$$

we average it over the electron coordinate $\mathbf{r}$ and then use the multipole expansion. The following integration over $\boldsymbol{\rho}$ and $\hat{\mathbf{R}}$ reduces the matrix element (6) to the multiple finite sum.

In the present study we restrict the basis set to the open channels only. Then, the boundary conditions at $R \to \infty$ for the radial functions contain ingoing and outgoing waves in the entrance channel and outgoing waves in all the other channels. The coupled differential equations (5) are solved numerically by Numerov method. In fact, we solve the equations with the standing-wave boundary conditions involving the real and symmetrical K-matrix instead of the S-matrix. The corresponding T-matrix is given by the equation $T = 2K/(I - iK)$, where I is the unit matrix. With the calculated T-matrix, one can obtain the cross sections of all the processes (1). In this paper we discuss the l-averaged $(n \to n')$ cross sections

$$\sigma_{n\to n'}(E) = \frac{\pi}{k_n^2 n^2} \sum_{l l' JLL'} (2J+1) |T_{nlL\to n'l'L'}^J|^2, \quad (7)$$

and the total CD cross sections

$$\sigma_n^{\mathrm{CD}}(E) = \sum_{n'<n} \sigma_{n\to n'}(E). \quad (8)$$

Results. The CC approach has been used to obtain the cross sections for the collisions of the $(\mu^- p)_n$ and $(\mu^- d)_n$ atoms with H atoms for $n = 3 \div 9$ at $E = 0.1 \div 100$ eV. The calculations of the CD cross sections for the given initial principal quantum number n were done with two sets of basis states: (a) the restricted basis including the states of two neighboring levels with $n' = n, n-1$ with all allowable l' (we refer these results, for brevity, as "two-level" approximation) and (b) the extended basis incorporating all the states with $n' \le n$. Notice that the CC two-level approximation, in some sense, is similar to the two-state approximations that were used by the previous authors [3–5].

In the both series of calculations the sums over the values of J in the cross sections are done until the accuracy better than 0.1% is reached at all energies. The analysis of the J dependence of the partial cross sections $\sigma_{nn'}^J$ shows that the main part of the CD cross sections comes from the partial waves with the relatively low J as compared with elastic scattering and Stark transitions. The same result was found in [5]. For example, for $n = 3$ and E_{cm} up to 100 eV we found for the CD process that $J_{\max}^{\mathrm{CD}} \le 15$ whereas for the elastic scattering $J_{\max}^{\mathrm{el}} \lesssim 120$. For the higher n the value $J_{\max}^{\mathrm{CD}}$ increases approximately $\sim \sqrt{n}$ and the interrelation between $J_{\max}^{\mathrm{CD}}$ and $J_{\max}^{\mathrm{el}}$ remains similar. This result is correlated with the relative importance of the different multipole terms of the interaction potential.

According to our study, the elastic scattering and Stark transitions can be with a good accuracy described within the CC method if to take into account only the long-range dipole terms in the matrix elements (6). In contrast, to provide the proper treatment of the CD all the allowed multipoles ($t \le t_{\max} = 2n - 2$) have to be included. For example, the CD cross section $\sigma_{6\to 5}$ at $E_{\mathrm{cm}} = 0.1$ eV calculated in "dipole" approximation is nearly twice as large as that obtained with all the multipoles included. Such a strong effect of the higher multipoles on the inelastic transitions is due to the fact that the main contribution to the inelastic transitions comes from small distances between colliding objects.

The CD cross sections of the $(\mu p) + H$ and $(\mu d) + H$ collisions in the two-level approximation are shown in Figs.1 and 2 together with the results of Bracci and Fiorentini [3] and Ponomarev and Solovyov [5], respectively. It is seen from Fig.1 that our two-level CC results are in satisfactory agreement with the results of the BF model [3] for $n = 5$, 7, 9, especially in the region $E_{cm} > 1$ eV. On the other hand, Fig.2 shows that our results for μd are by several times greater than the results obtained within the AA approach [5] for the transition $5 \to 4$ and even much greater (almost by two orders of

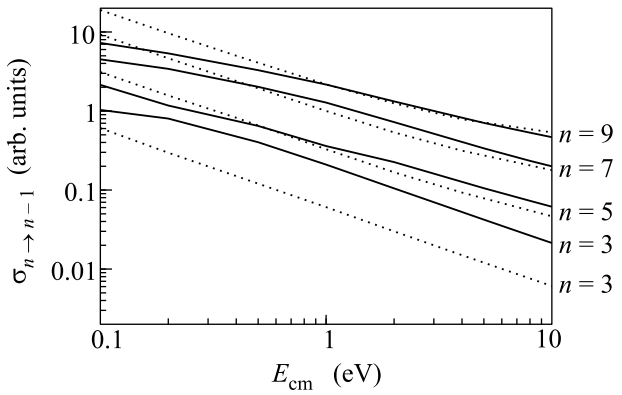

Fig.1. The CD cross sections $\sigma^{\rm CD}_{n,n-1}$ (a.u.) for $(\mu p)_n + H$ collisions with n =3, 5, 7, 9 calculated within CC two-level approximation (solid lines) in comparison with the results of Bracci and Fiorentini [3] (dotted lines)

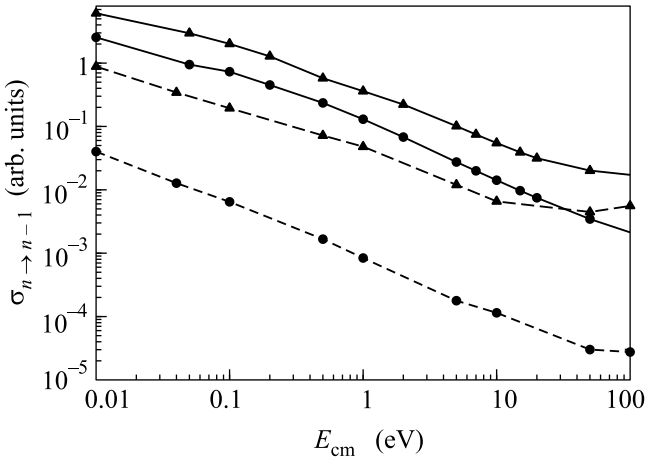

Fig.2. The cross sections of Coulomb deexcitation $\sigma^{\rm CD}_{n,n-1}$ (a.u.) for $(\mu d)_n + H$ collisions calculated within CC two-level approximation (solid lines) in comparison with the AA results [5] (dotted lines). The triangles and filled circles mark the curves for the $5 \to 4$ and $3 \to 2$ transitions, respectively

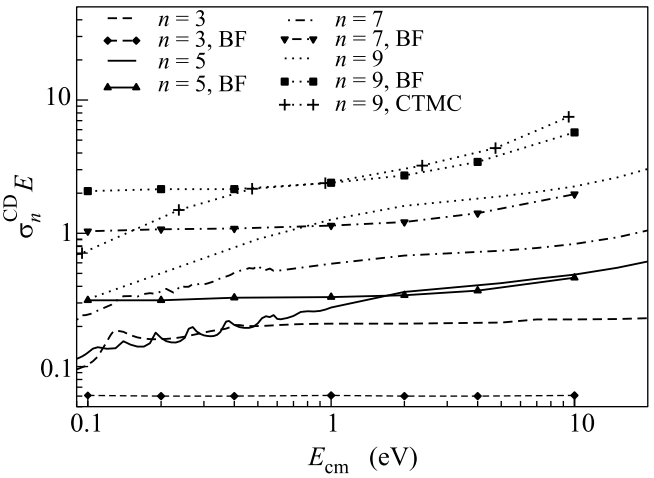

Fig.3. Energy dependence of the value $E \cdot \sigma^{\rm CD}_n(E)$ for different n in the $(\mu p)_n + H$ collisions obtained within the quantum CC approach (the curves without symbols) in comparison with the BF [3] (the curves with the triangles and squares) and CTMC [7] (the curve with crosses) results. The dashed, full, dot-dashed and dotted curves are for $n = 3$, 5, 7 and 9, respectively

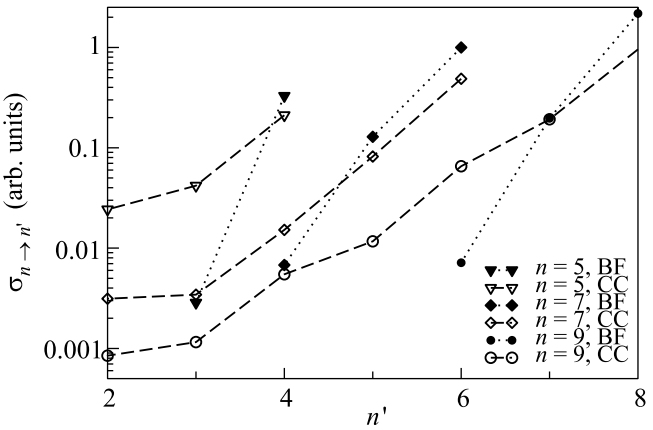

Fig.4. Dependence of the CD cross sections on the final principal quantum number n' for the different initial n in the $(\mu p)_n + H$ collisions at $E = 1$ eV. The dashed and dotted lines connect the points obtained in the present paper and in the [3], respectively. The triangles, squares and circles correspond to the initial $n = 5$, 7 and 9

magnitude) for the transition $3 \to 2$. The reason of this drastic discrepancy is not clear at present.

The results of the calculations with the extended basis set including all the states with $n' \le n$, are shown in Figs.3, 4 and Table. The comparison of these results with those obtained in the CC two-level approximation shows that the effect of the transitions with $\Delta n > 1$ on the CD cross sections is appreciable for $n \ge 4$. Moreover, the inclusion of the channels with $\Delta n > 1$ leads to a strong suppression of the main $\Delta n = 1$ transitions in comparison with the two-level CC approximation and due to this the total CD cross sections are also suppressed. For example, for $n = 4$ and 6 this suppression is about 1.5–2 and 3 times, respectively. As a result, the influence of the channels with $\Delta n > 1$ leads to an essential change of the E- and n-dependences as compared with the two-level CC calculation.

Beginning from the paper [3], it is commonly believed that the CD cross sections at low energies behave like $1/E$. In Fig.3 we show the total CD cross sections multiplied by energy that allows to reveal more explicitly the distinction from the $1/E$ behaviour. The present CD cross sections obtained within the extended basis are compared here with the results of the BF model [3] for

The CD cross sections $\sigma_{nn'}$ and $\sigma_n^{\rm CD}$ (in a.u.) for $(\mu p)_n + H$ collisions calculated in quantum-mechanical close-coupling approach

$E_{\rm cm}$, eV	0.1	0.2	0.5	1.0	2.0	5.0	7.0	10.0	15.0	20.0
$\sigma_3^{\rm CD}$	1.035	0.805	0.403	0.210	0.105	0.043	0.032	0.023	0.015	0.012
σ_{43}	0.936	0.704	0.515	0.333	0.189	0.083	0.060	0.043	0.030	0.024
σ_{42}	0.458	0.259	0.121	0.069	0.037	0.016	0.012	0.008	0.006	0.005
$\sigma_4^{\rm CD}$	1.397	0.965	0.637	0.403	0.226	0.098	0.071	0.052	0.036	0.029
σ_{54}	0.943	0.574	0.306	0.211	0.147	0.070	0.054	0.041	0.031	0.026
σ_{53}	0.219	0.164	0.074	0.042	0.022	0.009	0.007	0.005	0.003	0.003
σ_{52}	0.108	0.082	0.041	0.024	0.013	0.006	0.004	0.003	0.002	0.002
$\sigma_5^{\rm CD}$	1.270	0.819	0.422	0.277	0.182	0.085	0.065	0.049	0.037	0.031
σ_{65}	1.619	0.856	0.442	0.250	0.136	0.058	0.043	0.032	0.024	0.021
σ_{64}	0.440	0.270	0.178	0.115	0.064	0.028	0.021	0.016	0.012	0.010
σ_{63}	0.070	0.039	0.024	0.013	0.006	0.003	0.002	0.002	0.001	0.001
$\sigma_6^{\rm CD}$	2.166	1.189	0.661	0.387	0.211	0.090	0.067	0.050	0.038	0.033
σ_{76}	2.005	1.410	0.902	0.488	0.275	0.119	0.088	0.065	0.048	0.040
σ_{75}	0.354	0.279	0.136	0.082	0.054	0.024	0.019	0.014	0.011	0.010
σ_{74}	0.070	0.053	0.026	0.015	0.008	0.004	0.003	0.002	0.002	0.001
$\sigma_7^{\rm CD}$	2.454	1.762	1.076	0.591	0.340	0.148	0.111	0.083	0.062	0.053
σ_{87}	2.484	1.848	1.322	0.839	0.494	0.221	0.165	0.123	0.091	0.075
σ_{86}	0.396	0.294	0.186	0.128	0.084	0.037	0.028	0.021	0.016	0.013
σ_{85}	0.186	0.128	0.071	0.042	0.023	0.010	0.008	0.006	0.005	0.004
σ_{84}	0.031	0.018	0.010	0.006	0.003	0.001	0.001	0.001	0.001	0.001
$\sigma_8^{\rm CD}$	3.108	2.297	1.594	1.018	0.605	0.271	0.202	0.151	0.112	0.094
σ_{98}	2.070	1.773	1.319	0.956	0.604	0.287	0.221	0.170	0.131	0.114
σ_{97}	0.608	0.460	0.295	0.192	0.136	0.062	0.048	0.036	0.028	0.024
σ_{96}	0.294	0.191	0.106	0.065	0.037	0.017	0.013	0.010	0.008	0.008
σ_{95}	0.051	0.039	0.021	0.012	0.007	0.003	0.002	0.002	0.001	0.001
$\sigma_9^{\rm CD}$	3.055	2.486	1.754	1.233	0.789	0.371	0.285	0.220	0.170	0.148

$n = 3, 5, 7, 9$ and of the CTMC calculations by Jensen and Markushin [7] for $n = 9$. As it is seen from this figure, the energy dependence of the CC cross sections in the region $E > 1$ eV, as a whole, is in a qualitative agreement with the BF [3] and CTMC [7] models. But at lower energies the CC results don't confirm the $1/E$ energy dependence of the cross sections, except for the state with $n = 3$. At $E \lesssim 1$ eV and $n > 3$ our results show rather a $1/\sqrt{E}$ behaviour of the CD cross sections (the similar behaviour can be also seen in the CTMC results [7] for $n = 9$).

However, the more detailed insight reveals some resonance-like structures in energy behaviour of the CC cross sections at $E < 1$ eV (which are the most pronounced for $n = 5$ in Fig.3). This behaviour of the CD cross sections is due to the shape resonances in the entrance channel. The similar resonances at the same energy region have already been noted for the elastic scattering and Stark-transition cross sections obtained within the one-channel adiabatic approximation [8, 9].

The BF model predicts the power n-dependence nearly to n^γ with $\gamma > 2$. However, the present consideration doesn't confirm that the CD cross sections have such a scale factor depending on n (see Fig.3 and Table). Moreover, for $n = 4 \div 6$ the non-monotone behaviour of the $\sigma_n^{\rm CD}$ as a function of n is seen. A power dependence of the CD cross sections is found in the high energy region ($E > \varepsilon_n - \varepsilon_{n-1}$).

The dependence of the partial CD cross sections $\sigma_{n\to n'}$ on the final principal quantum number n' is shown in Fig.4 (see also Table). Our results for the distribution of the CD transitions over the final states n' are essentially different from the results of other approaches. The present calculations confirm that $\Delta n = 1$ transitions dominate in agreement with the previous results [3, 5, 7]. At the same time the transitions with $\Delta n > 1$ are strongly enhanced as compared to results [3, 5] and are in a satisfactory agreement with CTMC calculations [7]. The relative contribution of the transitions with $\Delta n > 1$ doesn't exceed 1% in AA approach [5], 10% in the BF model [3] and is about 19% in the CTMC calculations [7] (for $n = 9$). Our CC calculations of $\Delta n > 1$ transitions make up a substantial fraction of the total CD cross sec-

tions (16–37 %) for $n \geq 4$ and at all the energies under consideration.

Conclusion. We have studied the main features of the Coulomb deexcitation of excited (μp) and (μd) atoms in collision with H atom in the framework of the close-coupling approach. The present quantum-mechanical treatment of the CD process leads to the substantially new results in comparison with the previous studies, in particular:

– the transition $3 \to 2$ is strongly enhanced;

– the dominant transitions with $\Delta n = 1$ for $n \geq 4$ are essentially suppressed (about 2–3 and more times) for all energies under consideration;

– the fraction of the $\Delta n > 1$ transitions is very important and reaches up to 37%;

– the n-dependence of the CD cross sections is drastically changed;

– and, finally, the CD cross sections at $E \lesssim 1$ eV are suppressed and its behaviour is like $1/\sqrt{E}$.

The found gross features of CD process must take place for other exotic hydrogen atoms.

The obtained results are very important for the more realistic study of the kinetics and explanation of a high energy fraction of exotic hydrogen[1)]. The more detailed results will be published elsewhere.

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[1)] After this paper had been written we received the private communication from T. Jensen about results of his calculations of the density dependence of the relative K X-ray yields for muonic hydrogen. Using our data on the CD cross sections he obtain much better agreement with the experimental data.