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Scattering Processes of Excited Exotic Atoms: Close-Coupling Approach

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Motivation

We present quantum-mechanical calculations of non-reactive scattering processes of the excited exotic hydrogen-like atoms:

-elastic scattering

$$(ax)_n + (be^-)_{\nu} \to (ax)_n + (be^-)_{\nu};$$
 (1)

-Stark mixing

$$(ax)_{nl} + (be^{-})_{\nu} \to (ax)_{nl'} + (be^{-})_{\nu};$$
 (2)

Coulomb deexcitation

$$(ax)_{nl} + (be^{-})_{\nu} \to (ax)_{n'l'} + (b^{-}e)_{\nu}.$$
 (3)

Here a(b) = p, d, t (hydrogen isotopes); $x = \mu^{-}, \pi^{-}, K^{-}, \overline{p}$;

n, l are quantum numbers of exotic atom; ν are the hydrogen atom quantum numbers. The processes (1) - (2) decelerate while Coulomb deexcitation (3) accelerates the exotic atoms, influencing their quantum number and energy distributions during the cascade. The last process has attracted particular attention especially after the "hot" πp atoms with the kinetic energy up to 200 eV were found experimentally.

Hamiltonian

The non-relativistic Hamiltonian for the fourbody system $(a\mu^- + be^-)$ in Jacobi coordinates $(\mathbf{R}, \boldsymbol{\rho}, \mathbf{r})$:

$$H = -\frac{1}{2m}\Delta_{\mathbf{R}} + h_{\mu}(\boldsymbol{\rho}) + h_{e}(\mathbf{r}) + V(\mathbf{r}, \boldsymbol{\rho}, \mathbf{R}), \quad (4)$$

where m is the reduced mass of the system, h_{μ} and h_e are the Hamiltonians of the free exotic and hydrogen atoms:

$$h_{\mu}\Phi_{nlm}(\rho) = \varepsilon_n \Phi_{nlm}(\rho), \qquad (5)$$

$$h_e \varphi_{1s}(\mathbf{r}) = \epsilon_{1s} \varphi_{1s}(\mathbf{r}), \qquad (6)$$

and V is the interaction potential of the subsystems:

$$V(\mathbf{r}, \boldsymbol{\rho}, \mathbf{R}) = V_{ab} + V_{\mu b} + V_{ae} + V_{\mu e}$$
(7)

with the two-body Coulomb interactions

 $V_{ab} = |\mathbf{R} + \nu \boldsymbol{\rho} - \nu_e \mathbf{r}|^{-1}, V_{\mu b} = -|\mathbf{R} - \xi \boldsymbol{\rho} - \nu_e \mathbf{r}|^{-1}, (8)$ $V_{\mu e} = |\mathbf{R} - \xi \boldsymbol{\rho} + \xi_e \mathbf{r}|^{-1}, V_{ae} = -|\mathbf{R} + \nu \boldsymbol{\rho} + \xi_e \mathbf{r}|^{-1}. (9)$ The coefficients ν , ξ , ν_e and ξ_e in the two-body interactions (8)-(9) depend on the masses of the particles,

$$\nu = m_{\mu}/(m_{\mu} + m_a), \ \xi = m_a/(m_{\mu} + m_a), \ (10)$$

$$\nu_e = m_e/(m_e + m_b), \ \xi_e = m_b/(m_e + m_b), \ (11)$$

Coupled channel method

The total wave function $\Psi_E^{JM\pi}(\rho, \mathbf{r}, \mathbf{R})$ for the fixed values of J, M, π satisfied by the Schrödinger equation

$$(E-H)\Psi_E^{JM\pi}(\mathbf{r},\boldsymbol{\rho},\mathbf{R})=0,$$
 (12)

is expanded as follows

$$\Psi_E^{JM\pi}(\mathbf{r}, \boldsymbol{\rho}, \mathbf{R}) = \varphi_{1s}(\mathbf{r}) \frac{1}{R} \sum_{nlL} G_{nlL}^{J\pi}(R) |nl, L : JM\rangle.$$
(13)

This expansion leads to the coupled radial equations for the radial channel functions $G_{nlL}^{J\pi}(R)$:

$$\left(\frac{d^2}{dR^2} + k_n^2 - \frac{L(L+1)}{R^2}\right) G_{nlL}^{J\pi}(R)$$

= $2m \sum_{n'l'L'} W_{nlL,n'l'L'}^J(R) G_{n'l'L'}^{J\pi}(R),$ (14)

where $W^J_{nlL,n'l'L'}$ are the matrix elements of the interaction:

$$W^{J}_{nlL,n'l'L'} \equiv \langle \mathbf{1}s, nl, L : J | \hat{V} | \mathbf{1}s, n'l', L' : J \rangle.$$
 (15)

The radial functions $G_{E,n'l'L'}^{J\pi}(R)$ must be regular everywhere and satisfy the appropriate boundary conditions at $R \to 0$ and $R \to \infty$.

Cross sections

The partial cross sections of the processes (1) - (3) for the transitions $nl \rightarrow n'l'$

$$\sigma^{J}(nl \to n'l'; E) = \frac{\pi}{k_{i}^{2}} \frac{2J+1}{2l+1} \sum_{LL'} |T^{J}(nlL \to n'l'L')|^{2}.$$
(16)

The *l*-averaged partial cross sections for the transitions $n \rightarrow n'$ are then computed by summing over *l* and *l'* with the statistic factor $(2l+1)/n^2$:

$$\sigma_{n \to n'}^{J}(E) = \frac{\pi}{k_i^2} \frac{2J+1}{n^2} \sum_{l, l' LL'} |T^J(nlL \to n'l'L')|^2.$$
(17)

The total cross section for the transition $n \rightarrow n'$:

$$\sigma_{nn'}(E) = \sum_{J} \sigma_{nn'}^{J}(E).$$
(18)

Coulomb deexcitation cross sections



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The partial cross sections of the Coulomb deexcitation $\sigma_{3,2}^J$ and the elastic scattering $\sigma_{3,3}^J$ in a.u. for $(\mu p)_{n=3} + H$ collisions as function of the total angular momentum J at energies 0.1 eV, 2 eV and 50 eV.



The partial cross sections of the Coulomb deexcitation $\sigma_{7,6}^J$ (dashed) and the elastic scattering $\sigma_{7,7}^J$ (solid) in a.u. for $(\mu p)_{n=7} + H$ collisions as function of the total angular momentum J at energies 0.1 eV, 2 eV and 50 eV.



The cross sections of Coulomb deexcitation for $(\mu p)_n + H$ collisions calculated in the quantum-mechanical closecoupling method (solid lines) in comparison with the results of Bracci and Fiorentini (B&F – dashed) and classic Monte-Carlo results of Jensen and Markushin (J&M – dotted).



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 calculations (CC) and in the semiclassical approach by Bracci and Fiorentini (SC), respectively.



The total cross sections $\sigma_{nl \rightarrow nl'}$ for the collisions of the $p\bar{p}$ atom in the n = 8 state with hydrogen atom at $E_{\rm cm} = 1.4$ eV. The dashed and dotted lines connect the points corresponding to the calculations both with and without taking into account the *ns*-state energy shifts, respectively.



The *l*-averaged cross sections of the Stark transitions for the collisions of the $p\bar{p}$ atom with the hydrogenic one. The results of the calculations in the semiclassical model (SM) are shown for n = 8 with triangles



The *l*-averaged cross sections of Coulomb deexcitation with $\Delta n = 1, 2, 3$ for the collisions of the $p\bar{p}$ atom (n = 8) with the hydrogenic atom. The dashed line corresponds to the mass-scaling fit of the results of Bracci and Fiorentini for the muonic atom.

Differential cross sections



Differential elastic (a) and Stark (b) cross sections for $(\mu p)_{5l}$ + H collisions vs. cms scattering angle θ_{cm} at $E_{cm} = 1 \text{ eV}$.



Differential CD cross sections for the individual transitions with $\Delta n = 1$ (a) and $\Delta n = 2$ (b) for $(\mu p)_{n=5}$ +H collisions at $E_{cm} = 1$ eV



The *l*-average CD differential cross sections for the $6 \rightarrow 5$ transition in $(\mu p)_{n=6} + H$ collisions at different energies.

Effect of closed channels



Dependence of the Coulomb deexcitation cross sections $\sigma_{n\to n-1}$ for muonic and pionic hydrogen at $E_{\rm cm} = 1$ eV on the number of closed channels; n_{max} is the maximal principal quantum number of the included channels.