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Quantum-classical calculations of cascade transitions in hadronic hydrogen atoms

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Cascade processes in hadronic hydrogen:

radiative transitions :

$$(K^{-}x)_{nl} \to (K^{-}x)_{n'l'} + \gamma \qquad - \qquad (n' < n);$$

$$x = p, d$$

collisions :

$$(K^{-}x)_{nl} + X \to (K^{-}x)_{n'l'} + X \quad \begin{cases} \textit{elastic scattering}\ (n' = n,\ l' = l), \\ \textit{Stark transitions}\ (n' = n,\ l' \neq l), \\ \textit{Coulomb transitions}\ \ (n' \neq n), \end{cases}$$

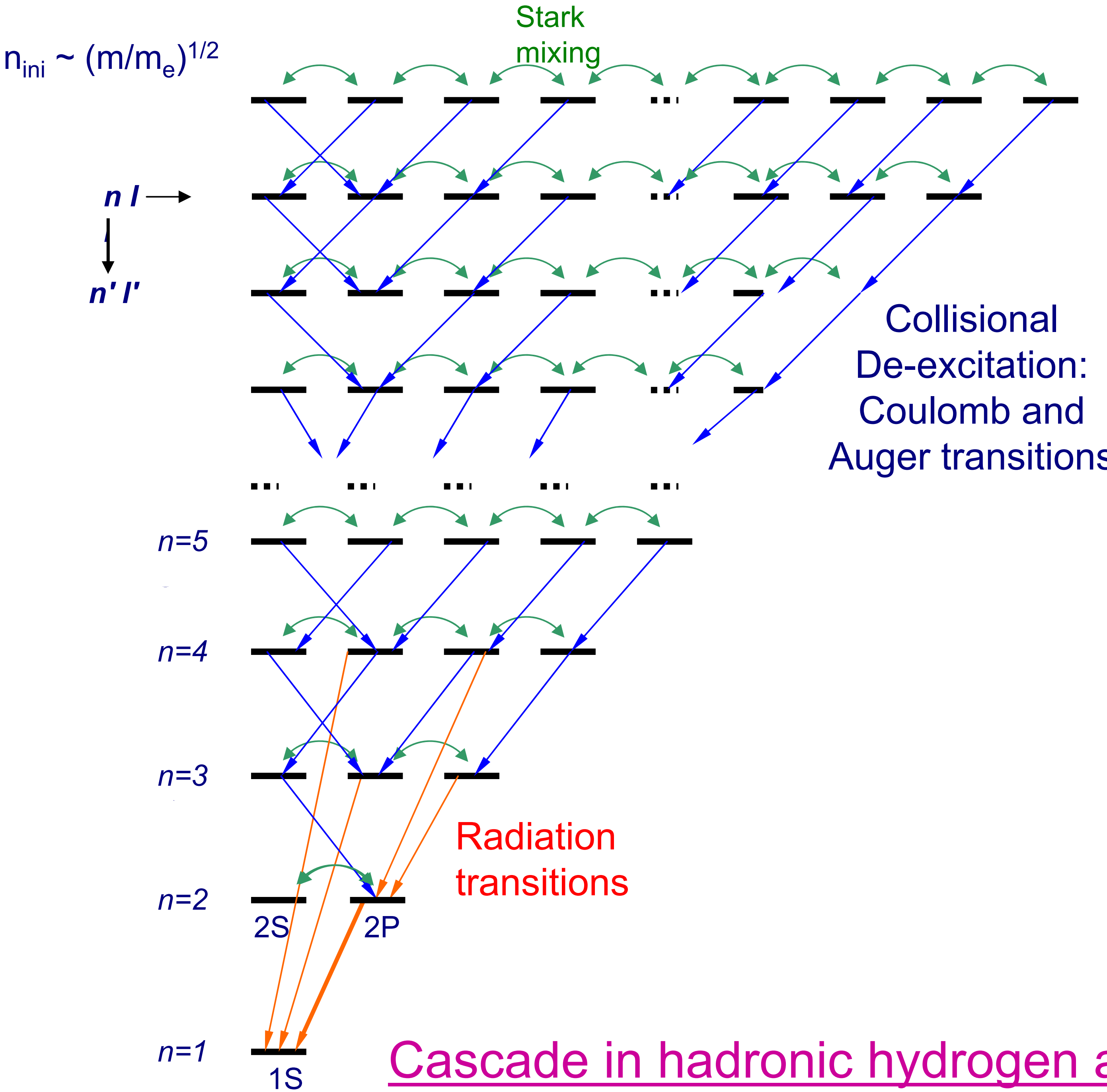
$$X = H, D$$

$$(K^{-}x)_{nl} + X \to (K^{-}x)_{n'l'} + x + e^{-} - \textit{Auger transitions}\ (n' < n),$$

$$(K^{-}x)_{nl} + X \to \left[(K^{-}x)_{n'l'}x\right] + e^{-} \quad - \textit{Auger capture}\ (n' < n),$$

$$\left[(K^{-}x)_{n'l'}x\right] \to (K^{-}x)_{n''l''} + x \qquad - \quad \textit{predissociation}\ (n'' < n').$$

Accompanying process : *nuclear absorption .*



Cascade in hadronic hydrogen atom

The general problem: *$(K^{-}x)_{nl} + X \rightarrow$ all final states*

The existing approaches to solve this problem:

Quantum Mechanics (QM) methods:

- three-body problem;
- multi-channel Coulomb problem (n^2~100÷1000 kaonic states);
- total and differential cross sections, the most part of which are lacking.

Classical Mechanics (CM) description:

- three planets problem (classical collisions);
- Coulomb charged planets, including the kaon motion;
- natural description of multi-quantum Coulomb transitions ($\Delta = n - n' > 1$);
- possibility to take into account protons chemical binding in H_2/D_2 molecule.

Good argument for solution of the QM problem by CM methods is successful description of electron charge exchange in collisions of multi-charged ions with hydrogen atoms (R. Olson and A. Salop, 1976): differences between calculated and experimental cross-sections are about ~20%.

Another argument is the Bohr Correspondence Principle: CM results coincide with QM ones at large n.

Quantum-Classical Monte Carlo method

Developed scheme of cascade calculations:

- **Radiative transitions are considered by QM methods;**
- **Collisions are described by methods of CM;**
- **Auger processes are treated semiclassically.**

The processes of Auger capture are negligible for heavy exotic atoms like $K^{-}p$ *and* $K^{-}d$, which become more and more energetic during the cascade due to multi-quantum Coulomb transitions.

The basic parameters of the problem:

The mean distances between hydrogen atoms: $\bar{R} = N^{-1/3} \approx 6\varphi^{-1/3} \gg 1,$

where $\varphi = N / N_0, \quad N_0 = 4.25 \cdot 10^{22}\, cm^{-3}\, (6 \cdot 10^{-3}\, a.u.).$

The radii of the Kepler kaon orbits $(n \sim 5)$: $r_n = n^2 / \mu \approx 4 \cdot 10^{-2},$

where $\mu = m_K m_x / (m_K + m_x).$

$$r_n \ll \bar{R}.$$

The "initial data sphere" radius: $R_0 = R_n + 2r_n; \quad R_n = 2 \div 5;$

The free path length: $\lambda_f = (\pi R_0^2 N)^{-1};$

The typical collision length: $\lambda_c \sim R_0;$

$$\frac{\lambda_f}{\lambda_c} = \frac{1}{\pi R_0^3 N} \approx \frac{50}{R_0^3 \varphi} \gg 1.$$

Free flight and

radiative transitions $(K^{-}x)_{nl} \to (K^{-}x)_{n'l'} + \gamma$

$$\lambda_f \gg \lambda_c ,$$

i.e., it is possible to neglect the radiative transitions during the collision.

The transitions $(nl) \to (n'l')$ are described by the quantum mechanical system of equations

$$\frac{dN_s(t)}{dt} = -\Gamma_s N_s(t) + \sum_{n'>n,l'} \Gamma_{s's} N_{s'}(t), \qquad \sum_{nl} N_s(t) = 1,$$

where $s \equiv (n,l), \quad \Gamma_s = \sum_{n'<n,l'} \Gamma_{s's}, \quad l' = l \pm 1.$

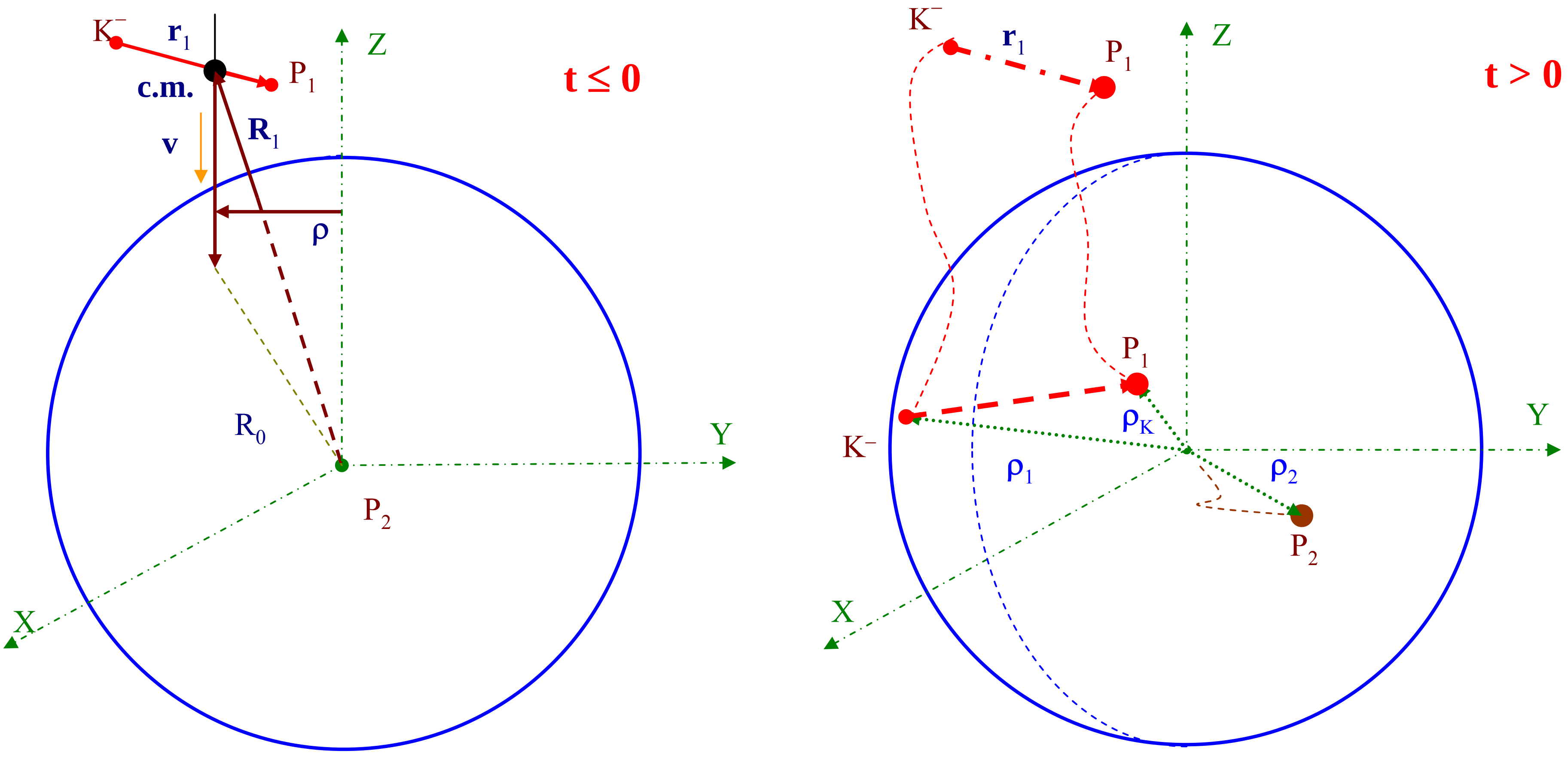
The initial conditions: $N_s(0) \equiv N_{nl}(0) = \delta_{nn_i} \delta_{ll_i}$.

The longevity of free flight: $t = \dfrac{1}{\pi R_0^2 N \mathrm{v}} \ln\left(\dfrac{1}{\xi}\right), \quad \xi \in (0,1).$

"Initial data" sphere

$\rho_1(t)$, $\rho_2(t)$, $\rho_K(t)$ – vector-coordinates of two protons and kaon;

ρ – impact parameter; $\mathbf{R}_1 = \mathbf{R}_{c.m.} - \rho_2$.



$(K^- p)_{nl} + H \rightarrow (K^- p)_{n'l'} + H$ -
3-body problem in Classical Mechanics

$$\begin{cases} m_K \dot{\mathbf{v}}_K = \mathbf{F}_{K1} + \mathbf{F}_{K2}, & \mathbf{F}_{12} = +\frac{1}{r_{12}^2} f(r_{12}) \hat{\mathbf{r}}_{12}, \quad \hat{\mathbf{r}}_{\mathbf{12}} = \frac{\mathbf{r}_{12}}{r_{12}}, \\ m_1 \dot{\mathbf{v}}_1 = -\mathbf{F}_{K1} + \mathbf{F}_{12}, & \mathbf{F}_{K1} = -\frac{1}{r_{K1}^2} f(\rho_{K1}) \hat{\mathbf{r}}_{K1}, \quad \hat{\mathbf{r}}_{K1} = \frac{\mathbf{r}_{K1}}{r_{K1}}, \\ m_2 \dot{\mathbf{v}}_2 = -\mathbf{F}_{K2} - \mathbf{F}_{12}, & \mathbf{F}_{K2} = -\frac{1}{r_{K2}^2} f(\rho_{K2}) \hat{\mathbf{r}}_{K2}, \quad \hat{\mathbf{r}}_{K2} = \frac{\mathbf{r}_{K2}}{r_{K2}}, \end{cases}$$

$$\rho_{K1} = \frac{r_{K1}^5}{\sigma}, \quad \rho_{K2} = \frac{r_{K2}^5}{\sigma}, \quad \sigma = r_{K1}^4 + r_{K2}^4, \quad \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j, \quad (i, j) = (1, 2, \mu).$$

$f(R) = (1 + 2R + 2R^2) e^{-2R}$ – the electron screening factor.

The initial conditions (at $t = 0$):

$$\mathbf{r}_\mu = \mathbf{R}_0 + \frac{m_1}{m_K} \mathbf{r}_{K1}, \quad \mathbf{r}_1 = \mathbf{R}_0 - \frac{m_K}{m_1} \mathbf{r}_{K1}, \quad \mathbf{r}_2 = 0,$$

$$\dot{\mathbf{r}}_\mu = \mathbf{v} + \frac{m_1}{m_K} \mathbf{v}_{K1}, \quad \dot{\mathbf{r}}_1 = \mathbf{v} - \frac{m_K}{m_1} \mathbf{v}_{K1}, \quad \dot{\mathbf{r}}_2 = 0.$$

The end of collision stage: fulfilment of the condition $r_{12} > R_0$.

As a results the transiiton $(n_i, l_i, E_i) \to (n_f, l_f, E_f)$ takes place:

$$n_f = \sqrt{-\frac{\mu}{2\varepsilon}}, \quad l_f = |\mathbf{l}_f|, \quad \varepsilon = \frac{\mu \dot{\mathbf{r}}_{K1}^2}{2} - \frac{1}{r_{K1}},$$

$$\mathbf{l}_f = \begin{cases} \mathbf{r}_{K1} \times \mu \dot{\mathbf{r}}_{K1}, \text{ if the final state is the } K^- p_1 - \text{atom}, \\ \mathbf{r}_{K2} \times \mu \dot{\mathbf{r}}_{K2}, \text{ if the final state is the } K^- p_2 - \text{atom}, \end{cases}$$

$$E_f = \begin{cases} \dfrac{m_{K1}}{2} \left(\dfrac{m_K \dot{\mathbf{r}}_K + m_1 \dot{\mathbf{r}}_1}{m_{K1}} \right)^2, \quad \text{for the } K^- p_1 - \text{atom}, \\[2ex] \dfrac{m_{K2}}{2} \left(\dfrac{m_K \dot{\mathbf{r}}_K + m_2 \dot{\mathbf{r}}_2}{m_{K2}} \right)^2, \quad \text{for the } K^- p_2 - \text{atom}, \end{cases}$$

Auger processes $(K^{-}p)_{nl} + H \to [(K^{-}p)_{n'l'} + p] + e$

The rate $\Gamma_n^A(R)$ of Auger transition:

$$\Gamma_n^A(R) = \frac{1{,}1 n^{11/2}}{\mu^{5/2}} \psi^2(R), \quad \text{at } n < n_0,$$

$$\Gamma_n^A(R) = \Gamma_{n_0}^A(R), \quad \text{at } n > n_0,$$

$$\psi^2(R) = \frac{e^{-2R}}{\pi}, \quad n = (\mu / I_H), \quad I_H \text{ is the hydrogen ionization energy}.$$

The probability of the Auger reaction:

$$W_A = 1 - \exp(-p_A),$$

$$\frac{dp_A}{dt} = \Gamma^A(r_{12}), \quad r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|.$$

At the moment $t = t_A$ of the Auger transition :

the electronic screening $f(R) = 1$, $n' = n - 1$, $l' = l - 1$.

A computational code for cascade processes in the exotic hydrogen atom

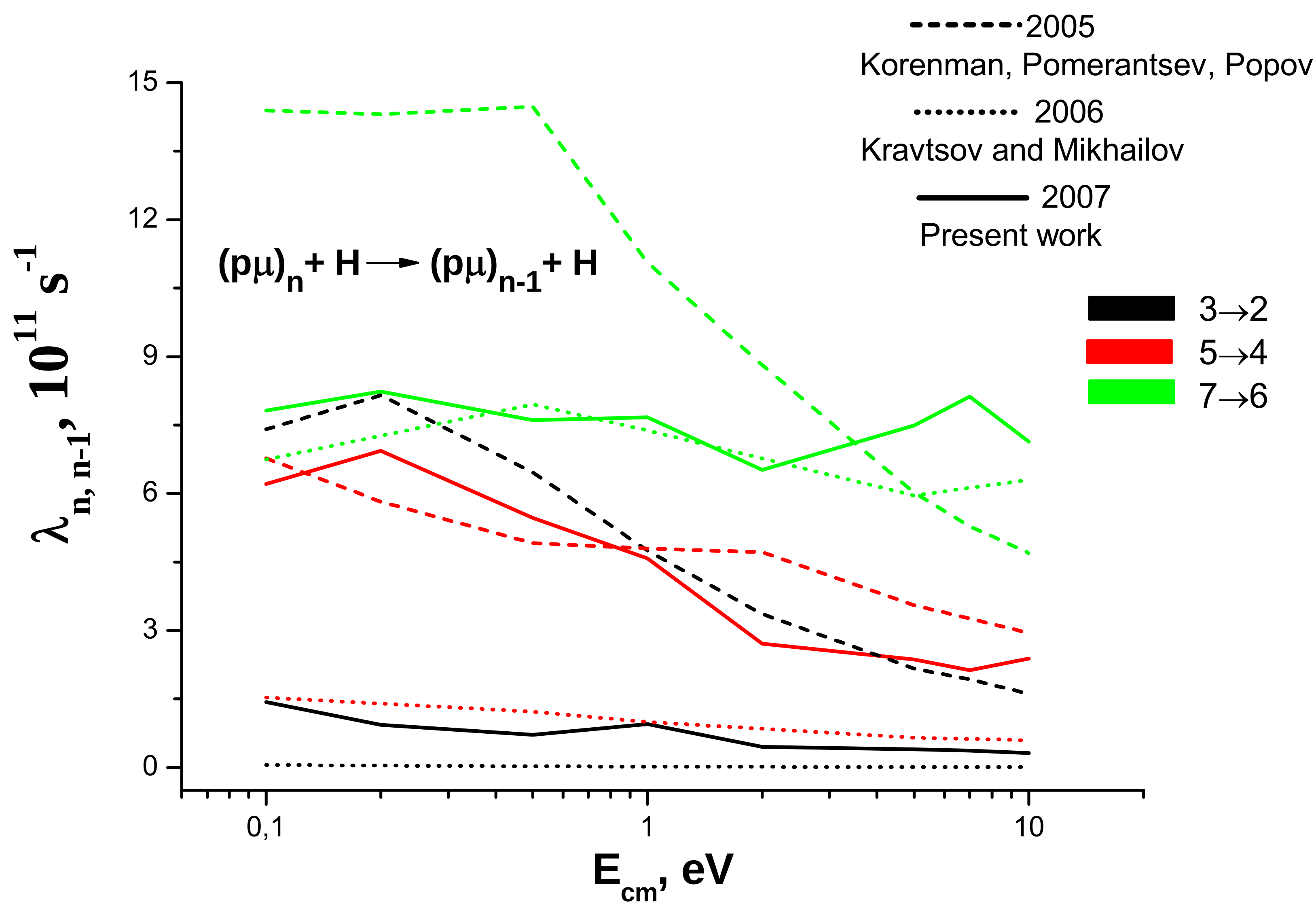
Input: an exotic atom in the {n,l,E} state.

Output: an exotic atom in the {n',l',E'} state,

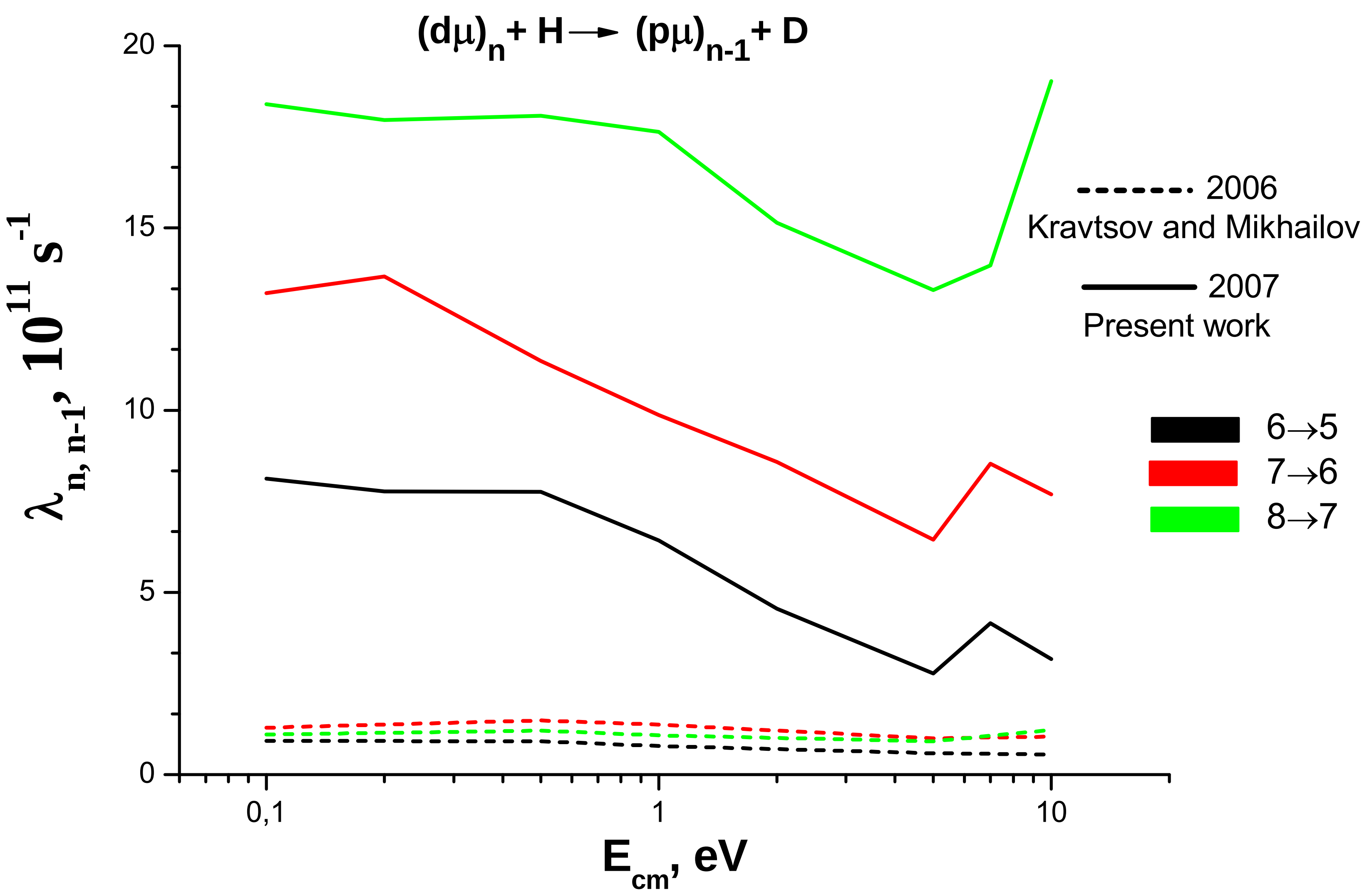
as well as,

- **cross-sections of Coulomb, Stark and Auger transitions;**
- **kinetic energy distributions;**
- **decay characteristics of the exotic molecular complex;**
- **cascade time in the exotic atom;**
- **Doppler broadening of the atomic {nl}-state;**
- **X-ray yields.**

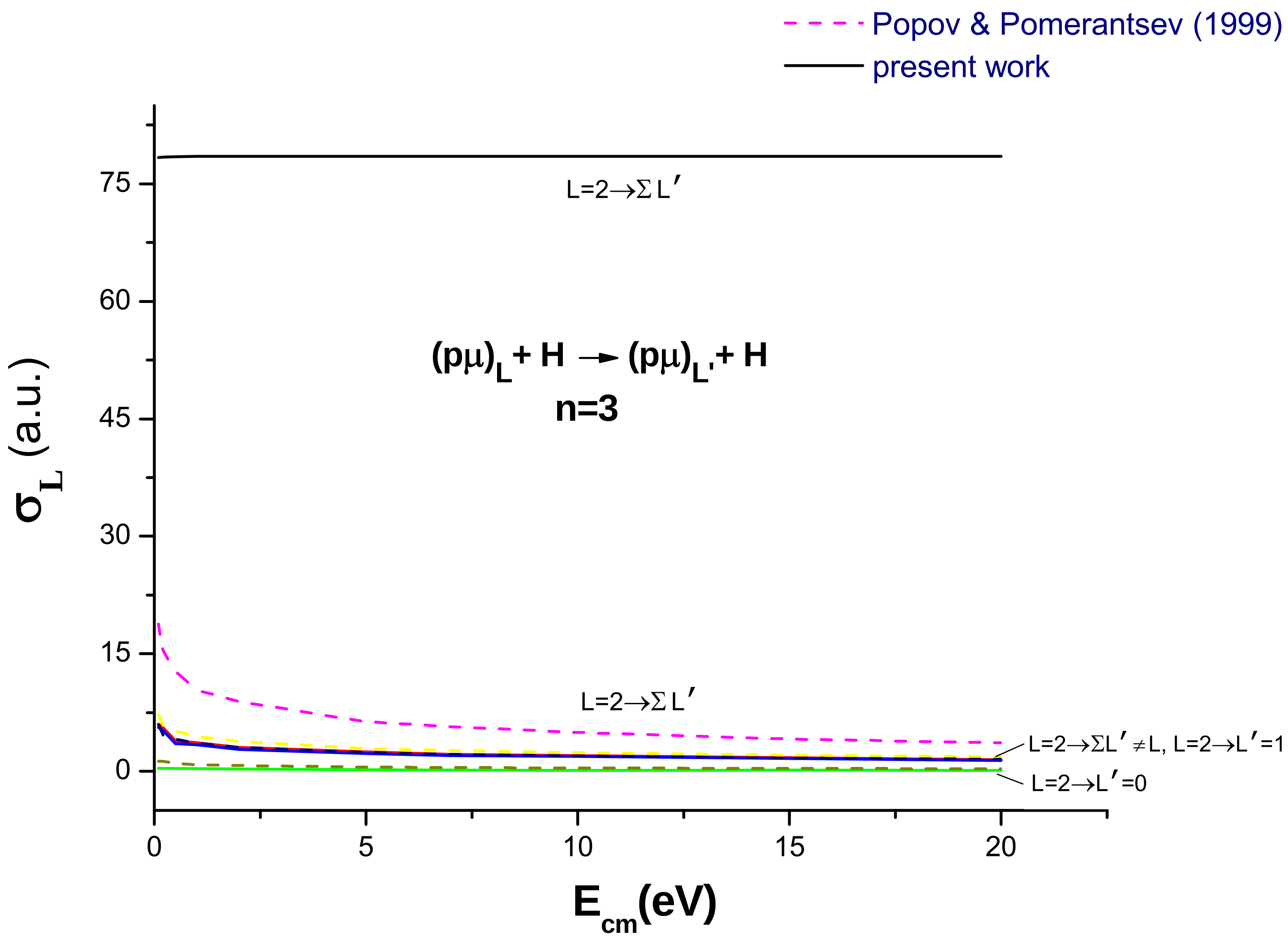
Coulomb de-excitation



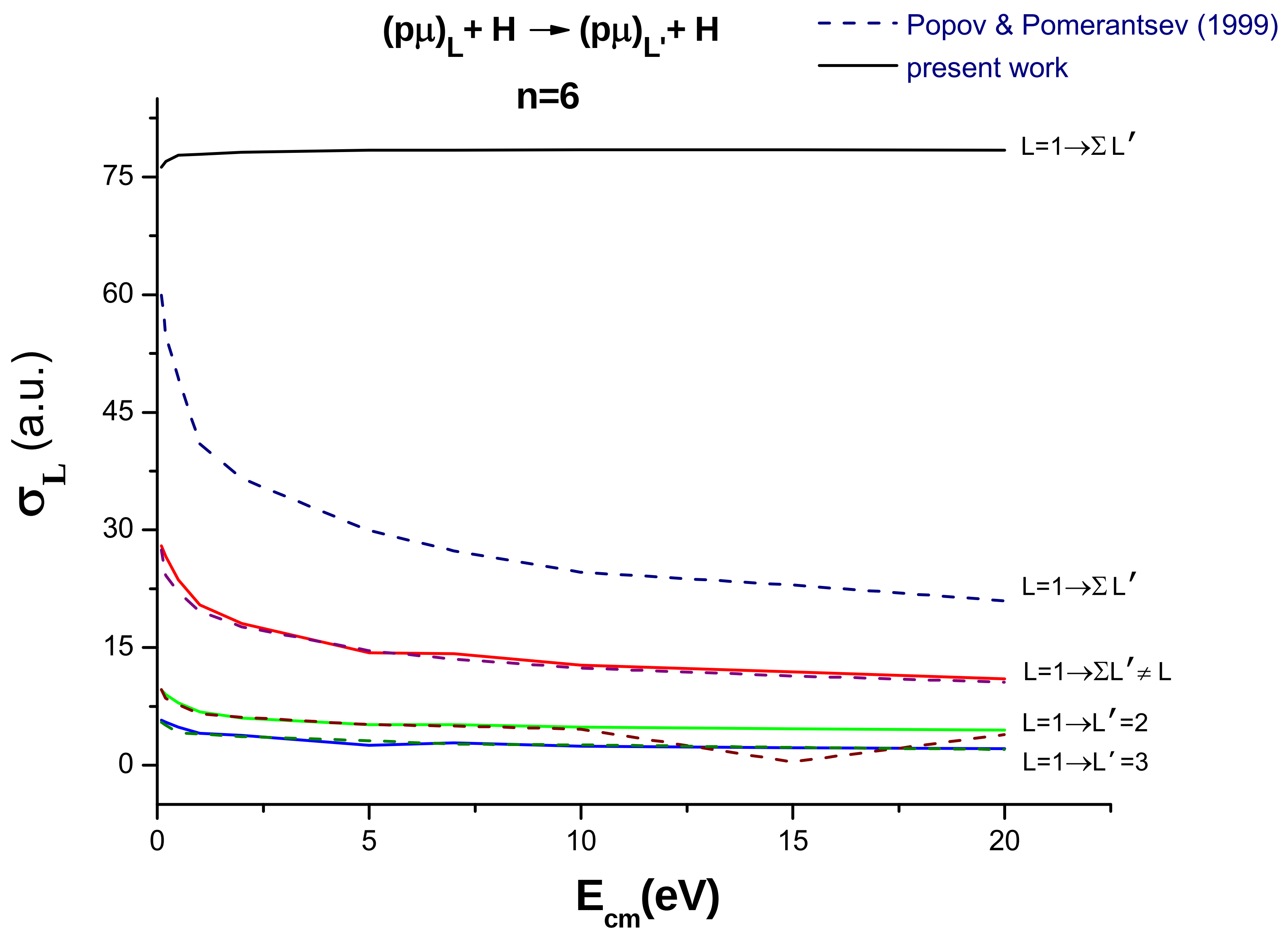
Charge exchange reaction



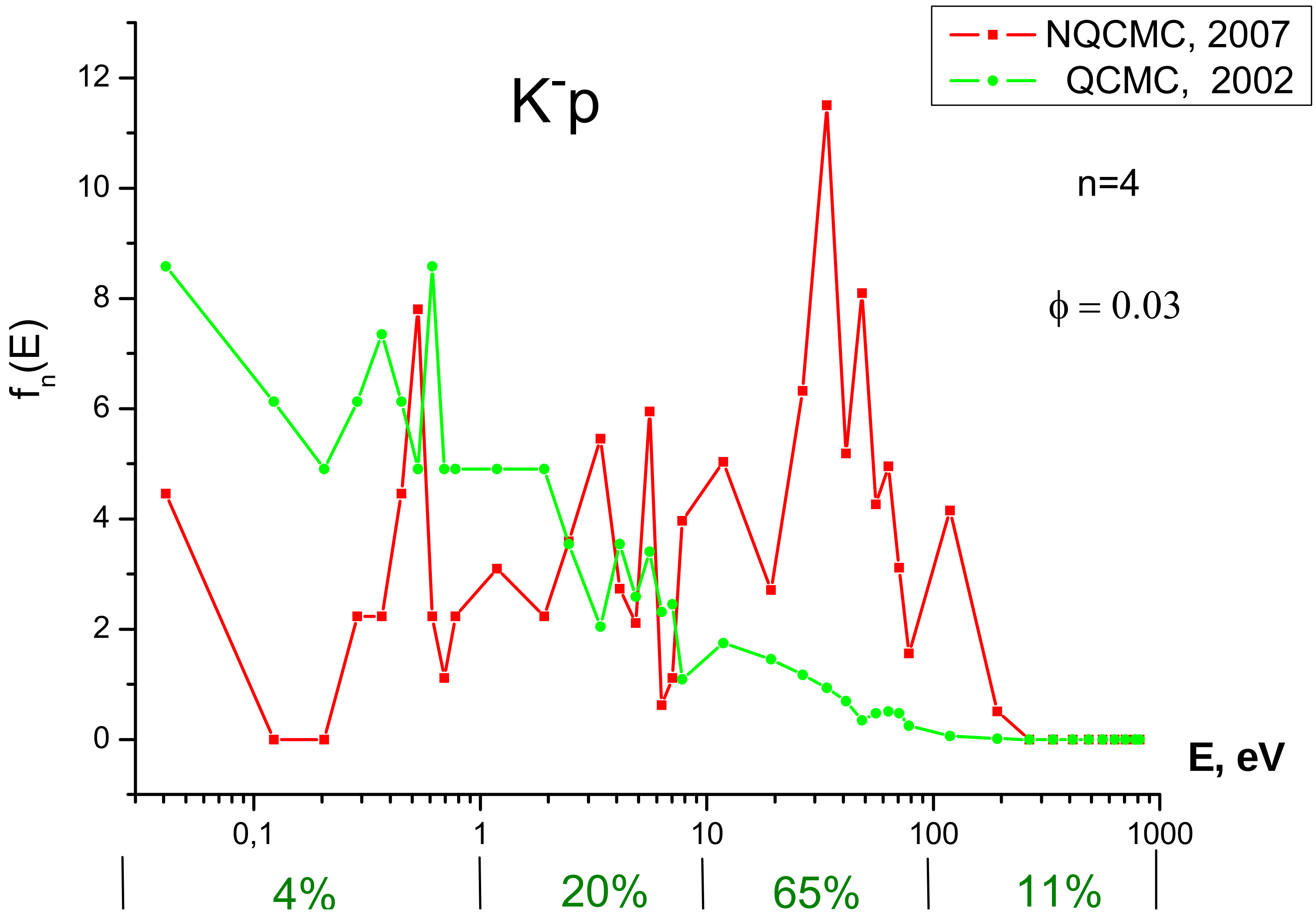
Stark collisions



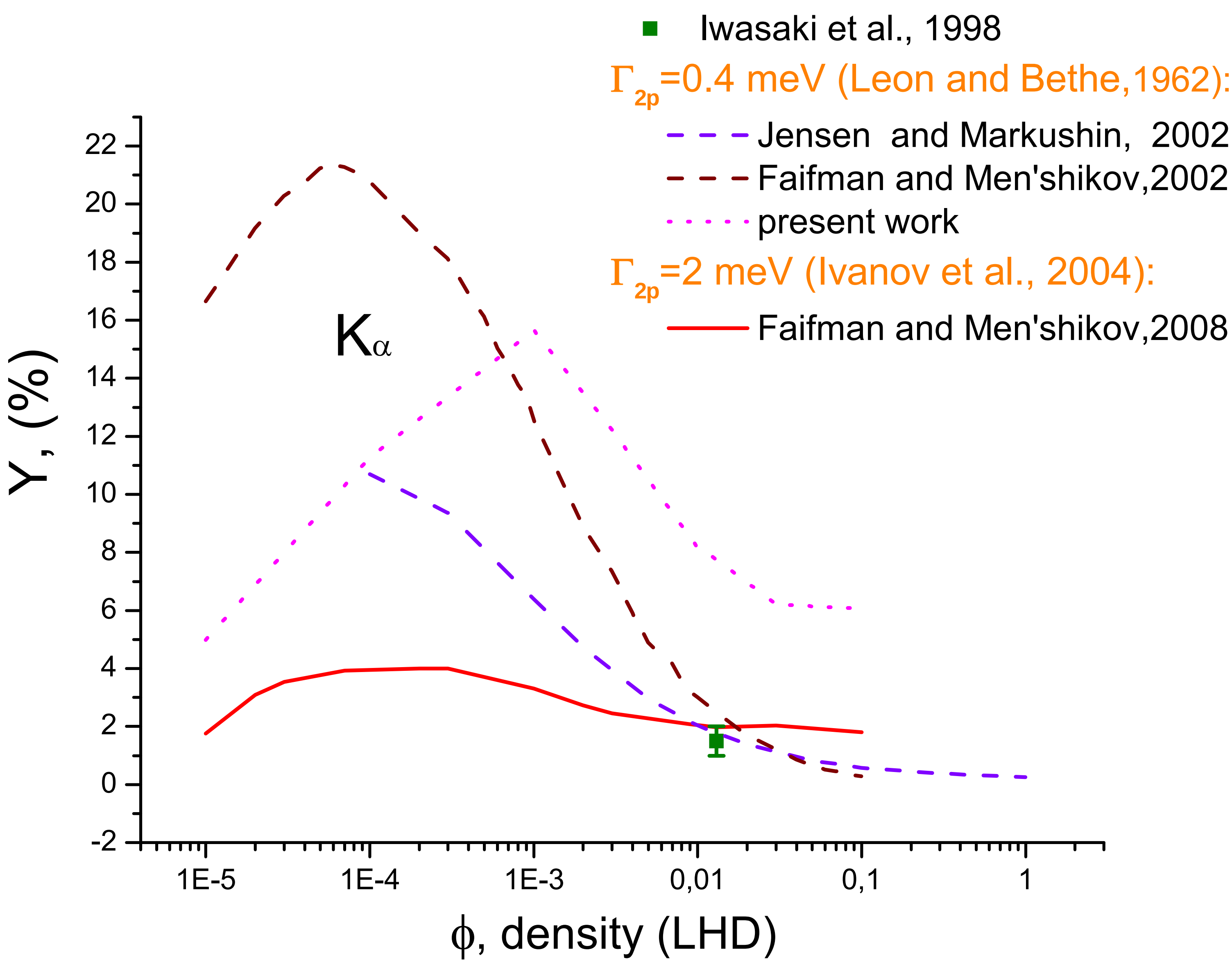
Stark collisions



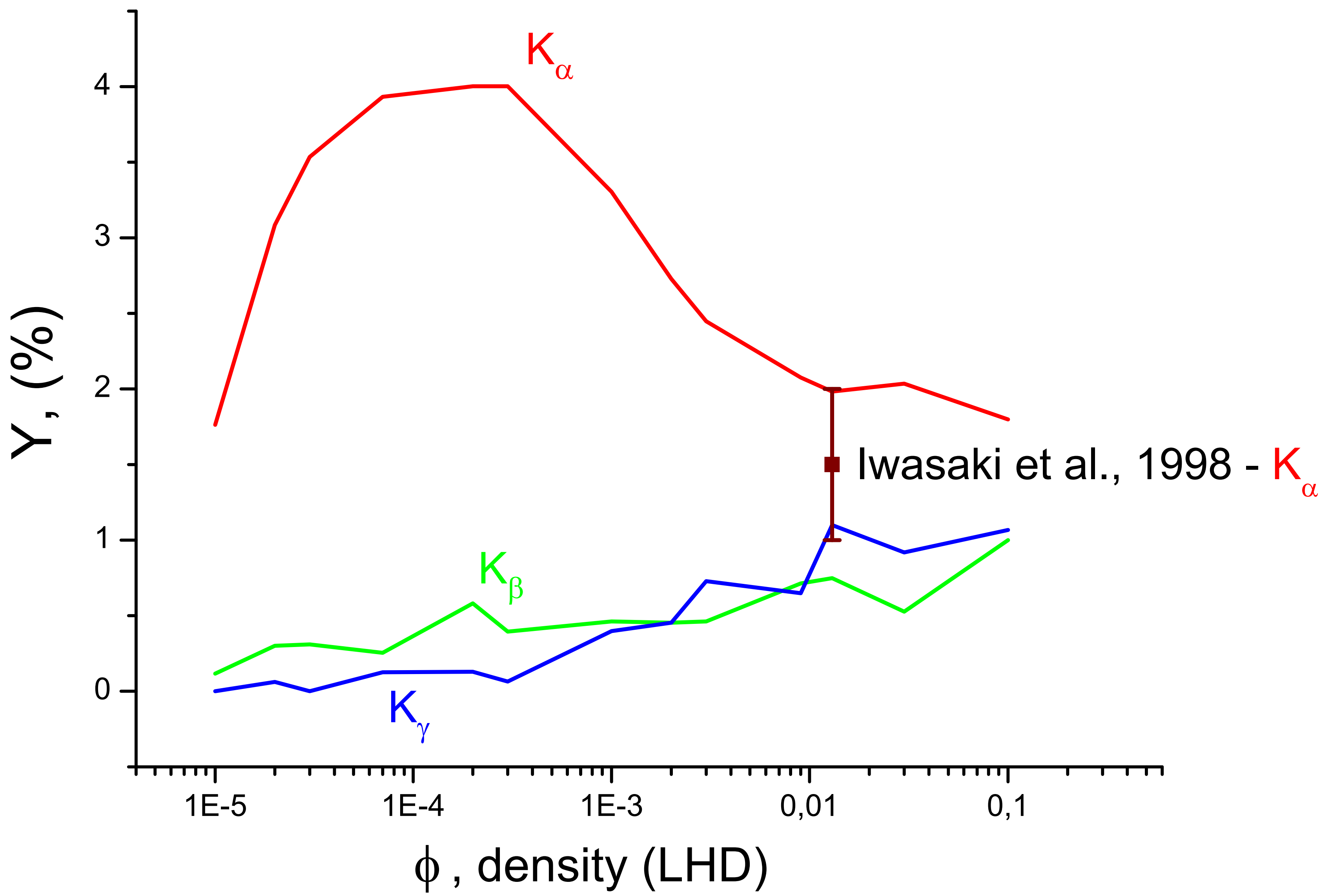
Fractions of pK⁻ atoms in the selected energy intervals



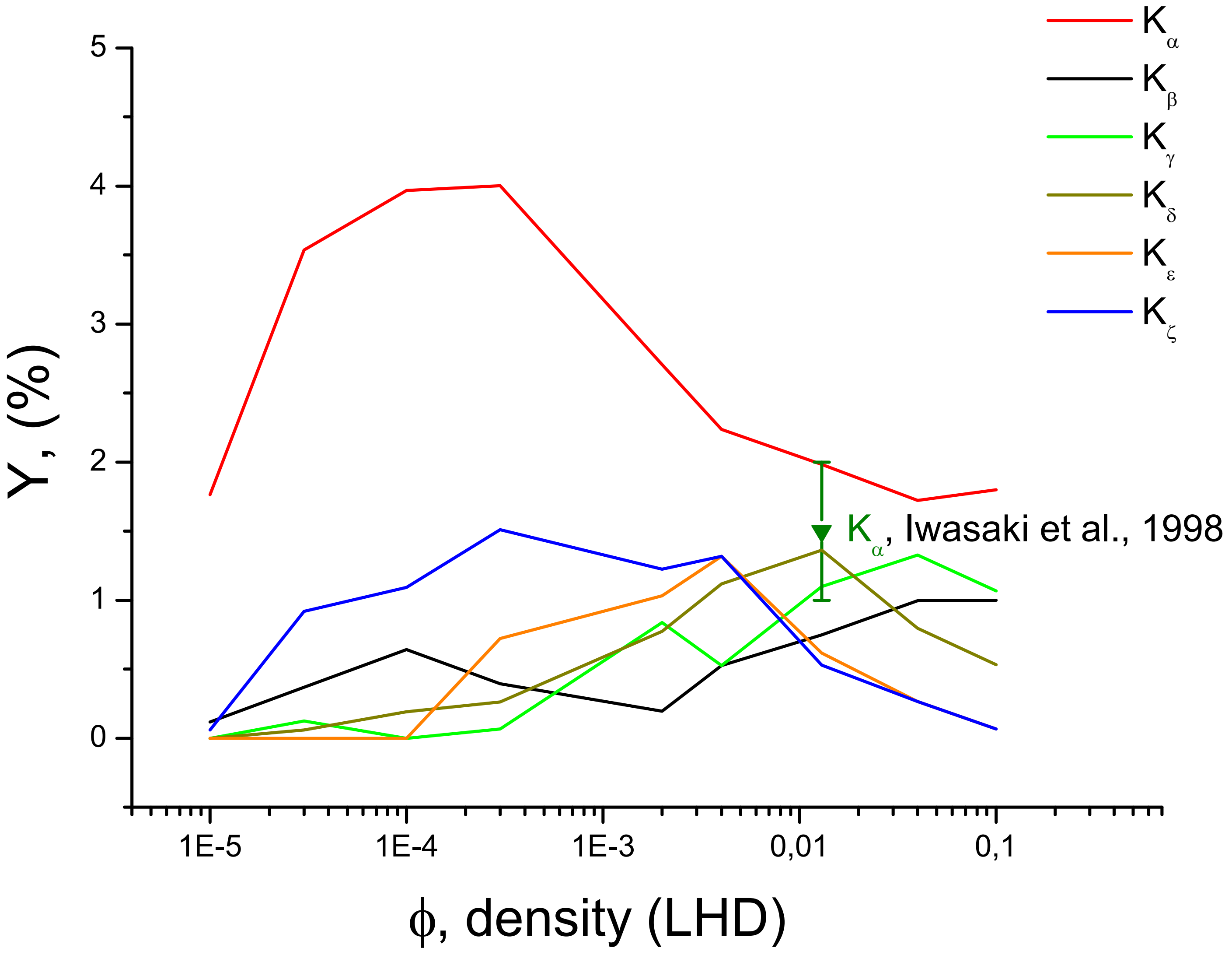
Calculated K_α-ray yields of K^-p atoms



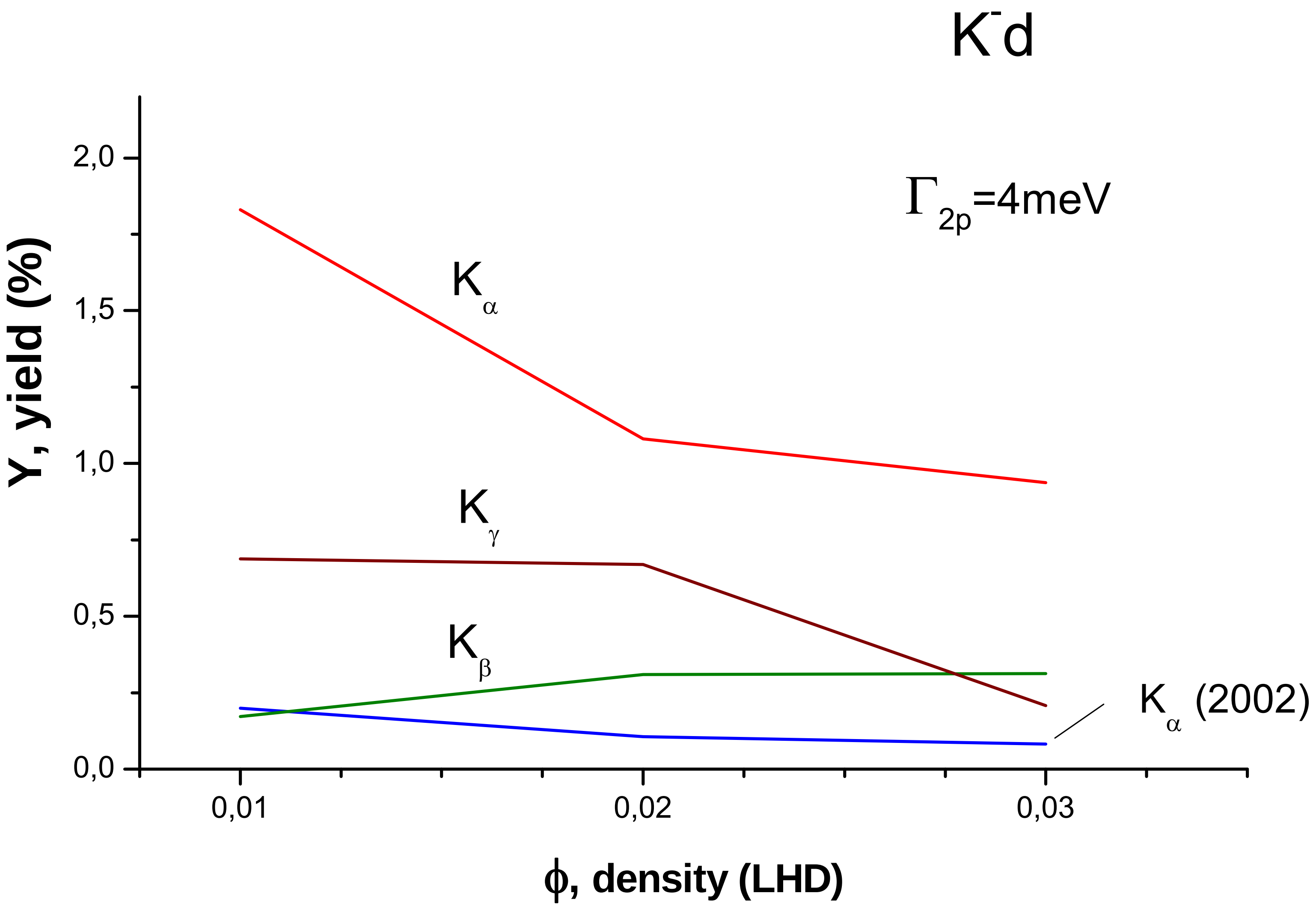
X-ray yields of kaonic hydrogen atoms



X-ray yields of kaonic hydrogen atoms



X-ray yields of kaonic deuterium atoms



Calculated $K_{x=\alpha,\beta,\gamma}$ yields of K^-d atoms at density ϕ=0.01 LHD

Γ_{2p} (meV)	Y_α (%)	Y_β (%)	Y_γ (%)
4	1,0 (0,2 - FM, 1999)	0,20	0
10	0,40	0	0,13
40	0,34	0	0

Summary

❖ A quantum-classical code for *ab initio* calculations of cascade in hadronic hydrogen atoms is developed.

❖ This code does not require any fit parameters.

❖ The obtained results have demonstrated good agreement between theory and available experimental data.

❖ The developed code enables to carry out calculations (with accuracy ~25% and less) of main characteristics of cascade processes:

- **cross-sections of Coulomb, Stark and Auger transitions;**
- **kinetic energy distributions;**
- **cascade time in the exotic atom;**
- **Doppler broadening of the atomic states;**
- **X-ray yields.**