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A Quantum-Classical Approach for the Study of Cascade Processes in Exotic Hydrogen Atoms

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The atom formation (initial stage): {pμ⁻, pK⁻} (n_0, l_0, E_0)

$$x^- + H \to (px^-)_{n_0 l_0 E_0} + e, \quad x^- = K^-, \mu$$

$$n_0 \sim \sqrt{\frac{m_x}{m_e}}, \quad n_0^{(\mu)} \approx 14, \quad n_0^{(K)} \approx 30, \quad W \approx \frac{2l_0+1}{n_0^2}, \quad E_0 \sim 1eV.$$

Cascade processes (de-excitation stages):

$$(px^-)_{nl} + H \to (px^-)_{n'l'} + H \quad \begin{cases} \text{elastic scattering } (n' = n, l' = l), \\ \text{Stark transitions } (n' = n, l' \neq l), \\ \text{Coulomb transitions } (n' \neq n), \end{cases}$$

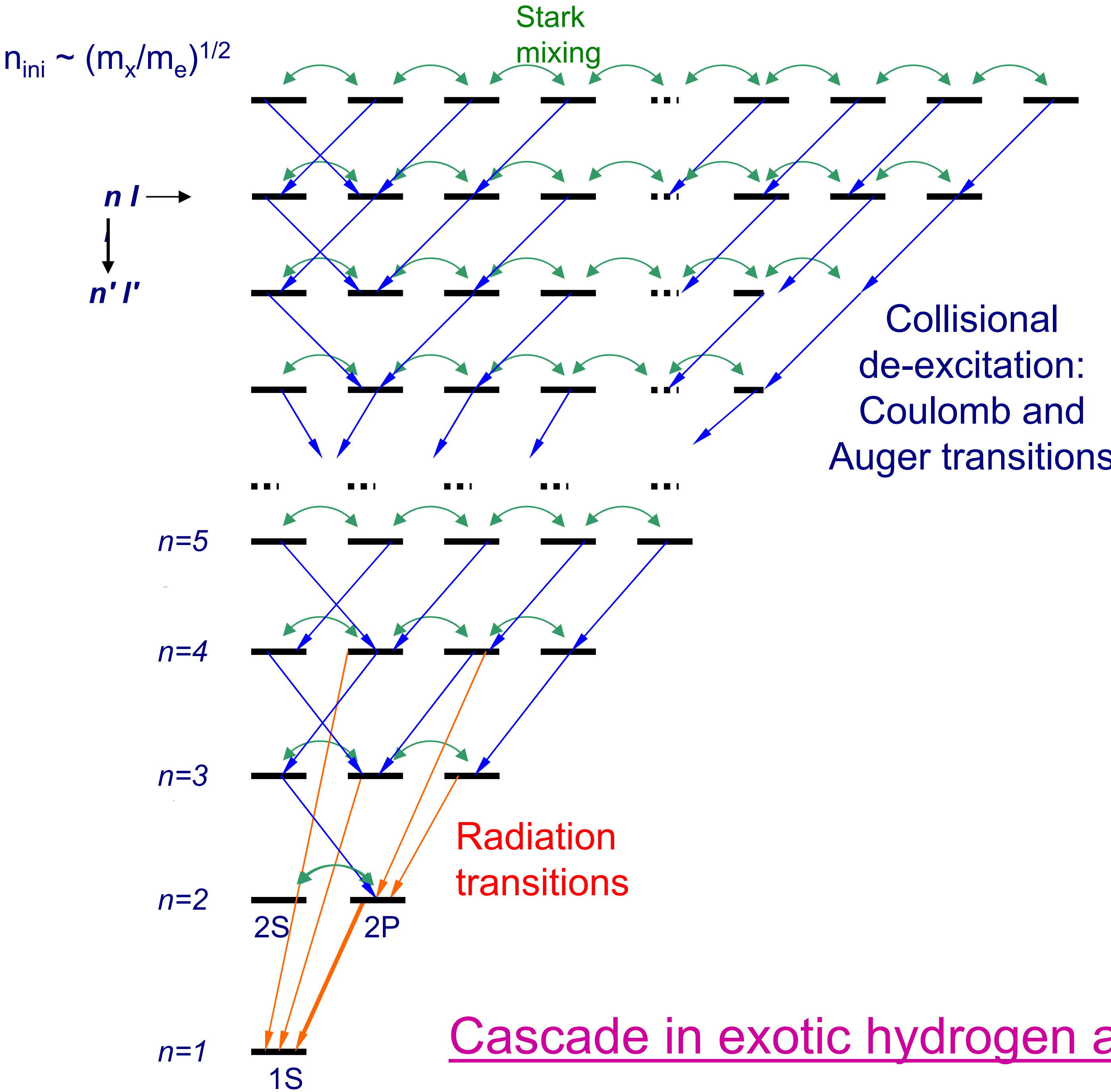
$$(px^-)_{nl} + H \to (px^-)_{n'l'} + p + e^- - \text{Auger transitions } (n' < n),$$

$$(px^-)_{nl} \to (px^-)_{n'l'} + \gamma \quad - \quad \text{radiative transitions } (n' < n).$$

Accompanying processes:

weak decay (μ⁻),

nuclear absorption (K⁻).



Cascade in exotic hydrogen atom

The general problem: $(px)_{nl} + H \to$ *all final states*

The existing approaches to solve this problem:

Quantum Mechanics (QM) methods:

- three-body problem;
- multi-channel Coulomb problem ($n^2 \sim 100 \div 1000$ muonic/kaonic states);
- total and differential cross sections (and the lack of the complete set of them).

Classical Mechanics (CM) description:

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

Good argument for solution of the QM problem by the CM methods is successful description of the 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: the CM results coincide with the same in QM at large n.

Mechanisms of $(px^-)_{nl}$ exotic atoms acceleration

$(px^-)_{nl}(E) + p \to (px^-)_{n'l'}(E') + p$ – *Coulomb transitions* $(n' < n,\ E' > E)$,

$(px^-)_{nl}(E) + H \to (px^-)_{n'l'}(E') + p + e^-$ – *Auger transitions* $(n' < n,\ \Delta = n_1 - n_2 \geq 0)$,

$(px^-)_{nl} + H \to C' + e^-,\ C' \equiv \left[(px)_{n'l'}\, p\right]$ – *Auger capture* $(n' = n - 1,\ \Delta = n_1 - n_2 < 0)$,

$C' \to C'' + \gamma,\quad C'' \equiv \left[(px)_{n''l''}\, p\right]$ – *radiative deexcitation* $(n' < n)$,

$C' \to (px)_{n''l''} + p$ – *predissociation* $(n'' < n' = n - 1)$.

Quantum-Classical Monte Carlo method

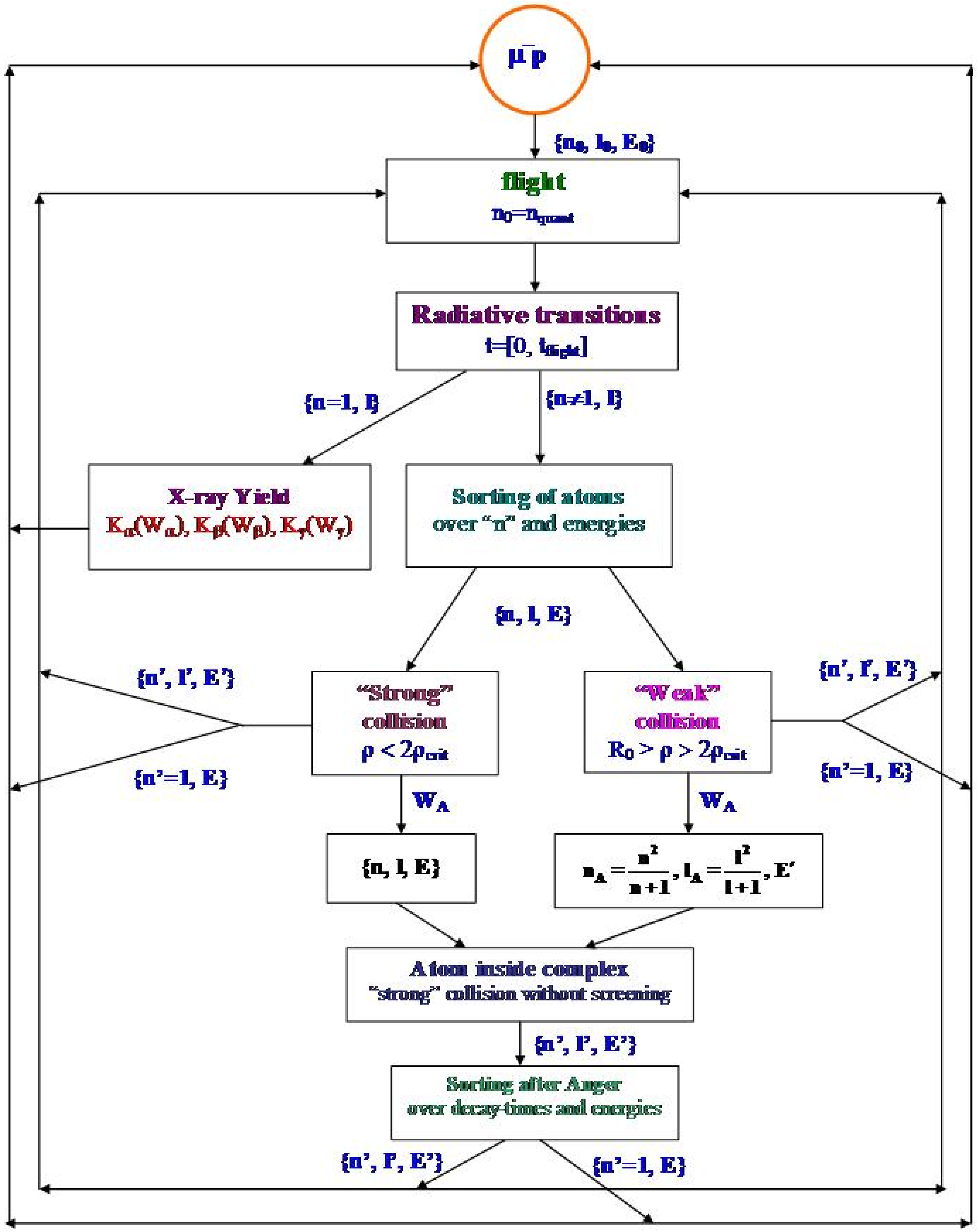
Proposed scheme of cascade calculations:

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

The processes of Auger capture are negligible for heavy exotic atoms (e.g., pK^-), which become more and more energetic during the cascade due to multi-quantum Coulomb transitions.

How Auger processes is important for light exotic atoms ($p\mu$)?

Block-scheme of the muonic atom cascade in hydrogen.



Block-scheme of exotic atom cascade in hydrogen

Output:

- 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.

The basic parameters of the problem:

The mean distances between 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 muon orbits $(n \sim 5)$: $r_n = n^2 / \mu \approx 0.15,$

where $\mu = m_\mu m_p / (m_\mu + m_p).$

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

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 $(p\mu)_{nl} \to (pm)_{n'l'} + \gamma$

λ_f » λ_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

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

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

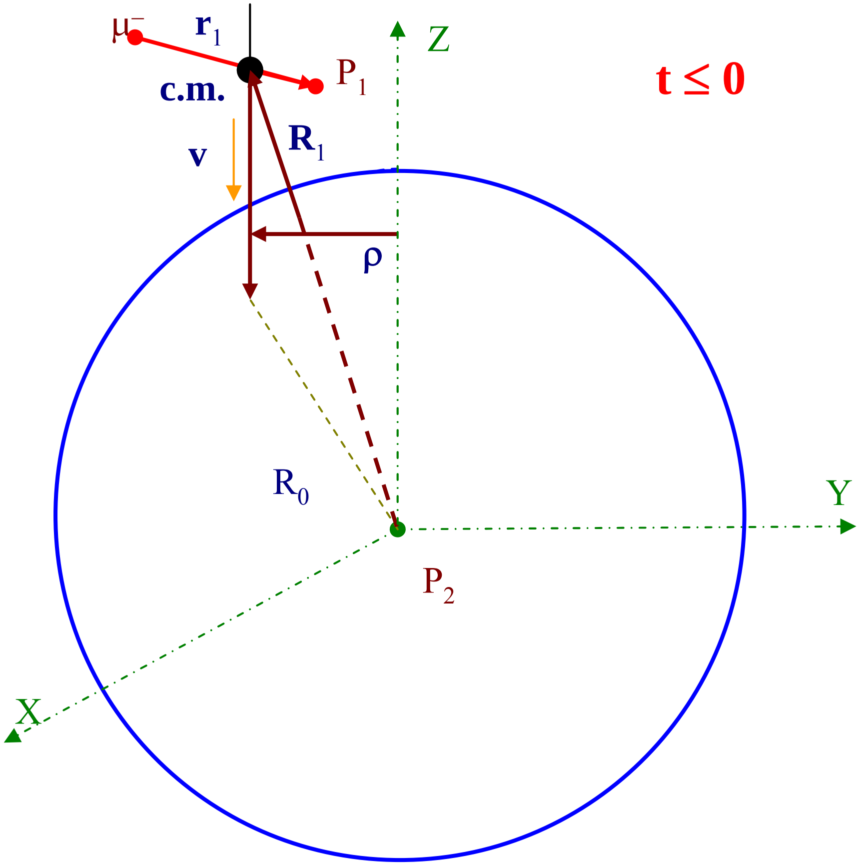
$$\text{The initial conditions: } N_s(0) \equiv N_{nl}(0) = \delta_{nn_i}\delta_{ll_i} \,.$$

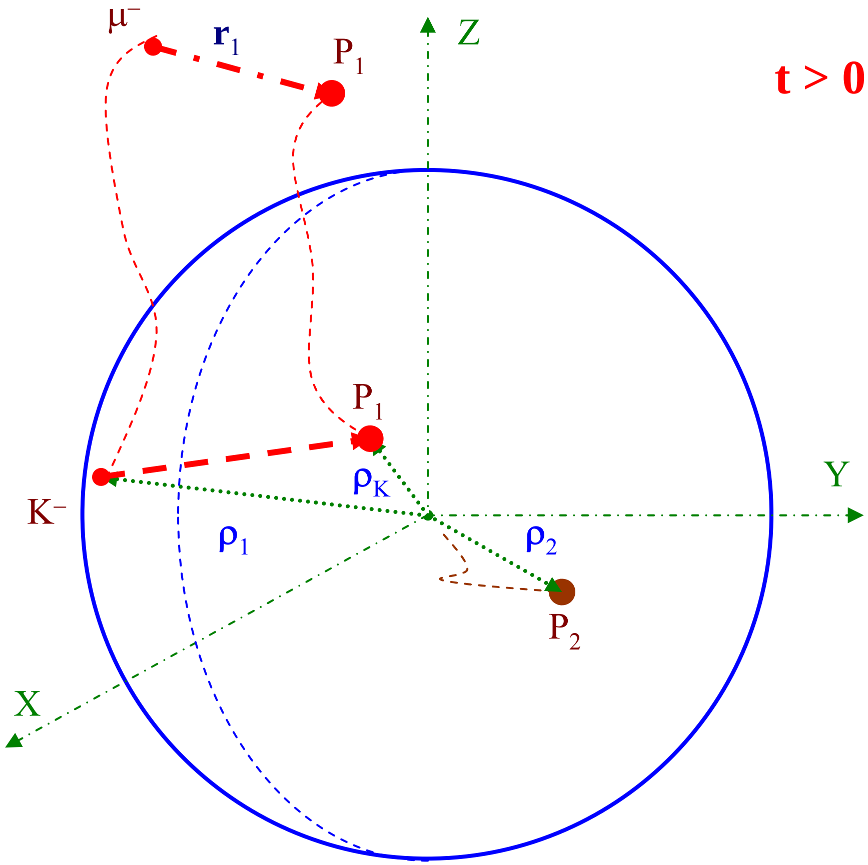
$$\text{The longevity of free flight: } t = \frac{1}{\pi R_0^2 N \mathrm{v}} \ln\left(\frac{1}{\xi}\right), \quad \xi \in (0,1).$$

“Initial data” sphere

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

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





$(p\mu)_{nl} + H \rightarrow (p\mu)_{n'l'} + H$ -

3-body problem in Classical Mechanics

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

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

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

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

$$
\mathbf{r}_\mu = \mathbf{R}_0 + \frac{m_1}{m_\mu}\mathbf{r}_{\mu 1}, \quad \mathbf{r}_1 = \mathbf{R}_0 - \frac{m_\mu}{m_1}\mathbf{r}_{\mu 1}, \quad \mathbf{r}_2 = 0,
$$

$$
\dot{\mathbf{r}}_\mu = \mathbf{v} + \frac{m_1}{m_\mu}\mathbf{v}_{\mu 1}, \quad \dot{\mathbf{r}}_1 = \mathbf{v} - \frac{m_\mu}{m_1}\mathbf{v}_{\mu 1}, \quad \dot{\mathbf{r}}_2 = 0.
$$

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

As a result the transition $(n_i, l_i, E_i) \rightarrow (n_f, l_f, E_f)$ takes place:

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

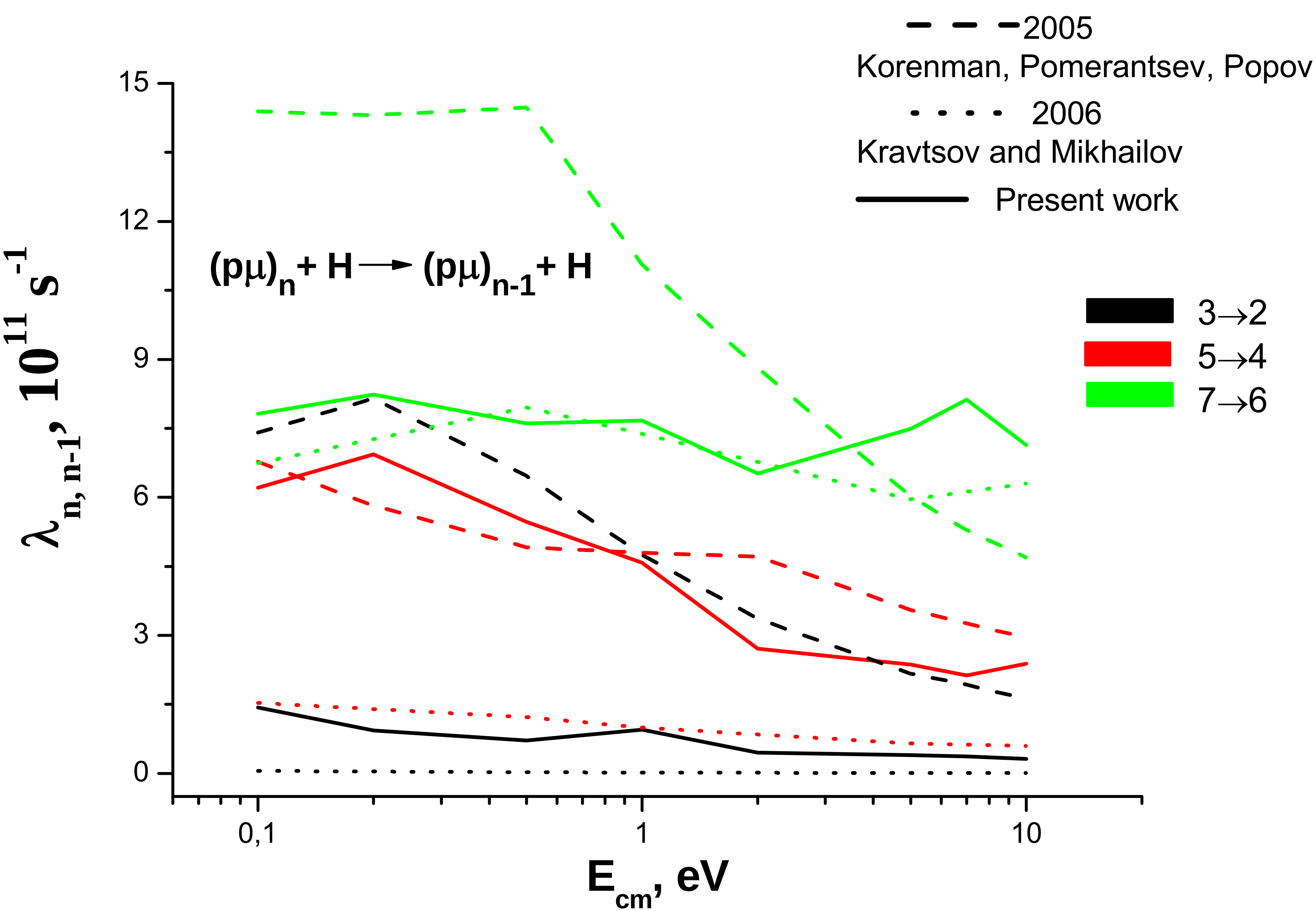
$$\mathbf{l}_f = \begin{cases} \mathbf{r}_{\mu 1} \times \mu \dot{\mathbf{r}}_{\mu 1}, \text{ if the final state is the } p_1\mu - \text{atom}, \\ \mathbf{r}_{\mu 2} \times \mu \dot{\mathbf{r}}_{\mu 2}, \text{ if the final state is the } p_2\mu - \text{atom}, \end{cases}$$

$$E_f = \begin{cases} \dfrac{m_{\mu 1}}{2} \left(\dfrac{m_\mu \dot{\mathbf{r}}_\mu + m_1 \dot{\mathbf{r}}_1}{m_{\mu 1}} \right)^2, \quad \text{for the } p_1\mu - \text{atom}, \\ \dfrac{m_{\mu 2}}{2} \left(\dfrac{m_\mu \dot{\mathbf{r}}_\mu + m_2 \dot{\mathbf{r}}_2}{m_{\mu 2}} \right)^2, \quad \text{for the } p_2\mu - \text{atom}, \end{cases}$$

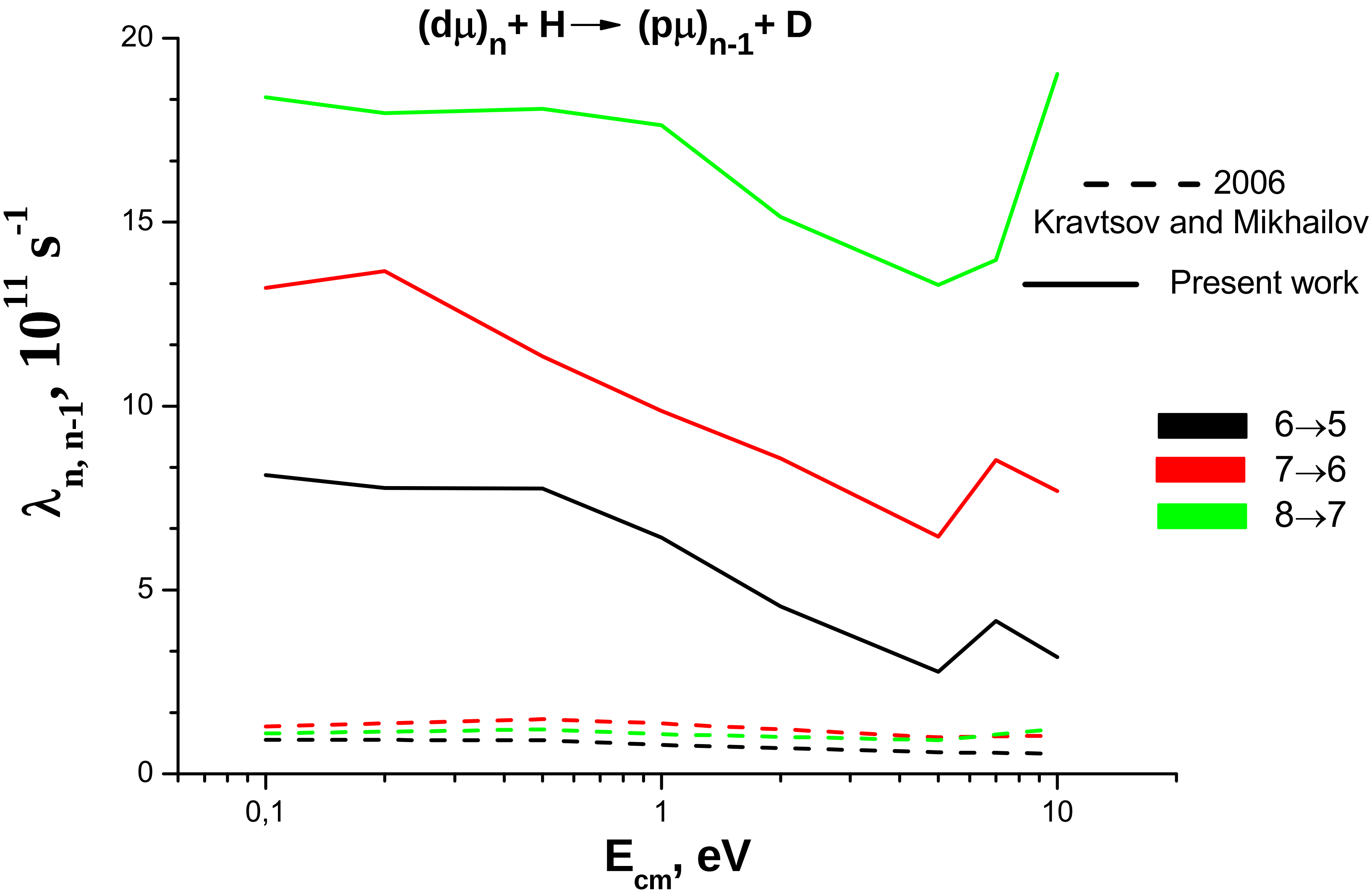
The rate of the Coulomb transition $n_i \rightarrow n_f$:

$$\lambda_{nn'} = N\text{v}\sigma_{nn'}; \qquad \sigma(n_i \rightarrow n_f) = \pi R_0^2 \sum_{l_i l_f} \frac{2l_i + 1}{n_i^2} \frac{N_{(nl)_i \rightarrow (nl)_f}}{N_{tot}}.$$

Coulomb de-excitation



Charge exchange reaction



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

The rate of Auger transition $\Gamma_n^A(R)$ $\left(\textit{theory by Bukhvostov and Popov}, 1982\right)$:

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

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

$$\psi^2(R) = \frac{e^{-2R}}{\pi}, \qquad n_0 = (\mu / I_H), \;\; I_H \textit{ is the ionization energy of } H.$$

The probability of the Auger process:

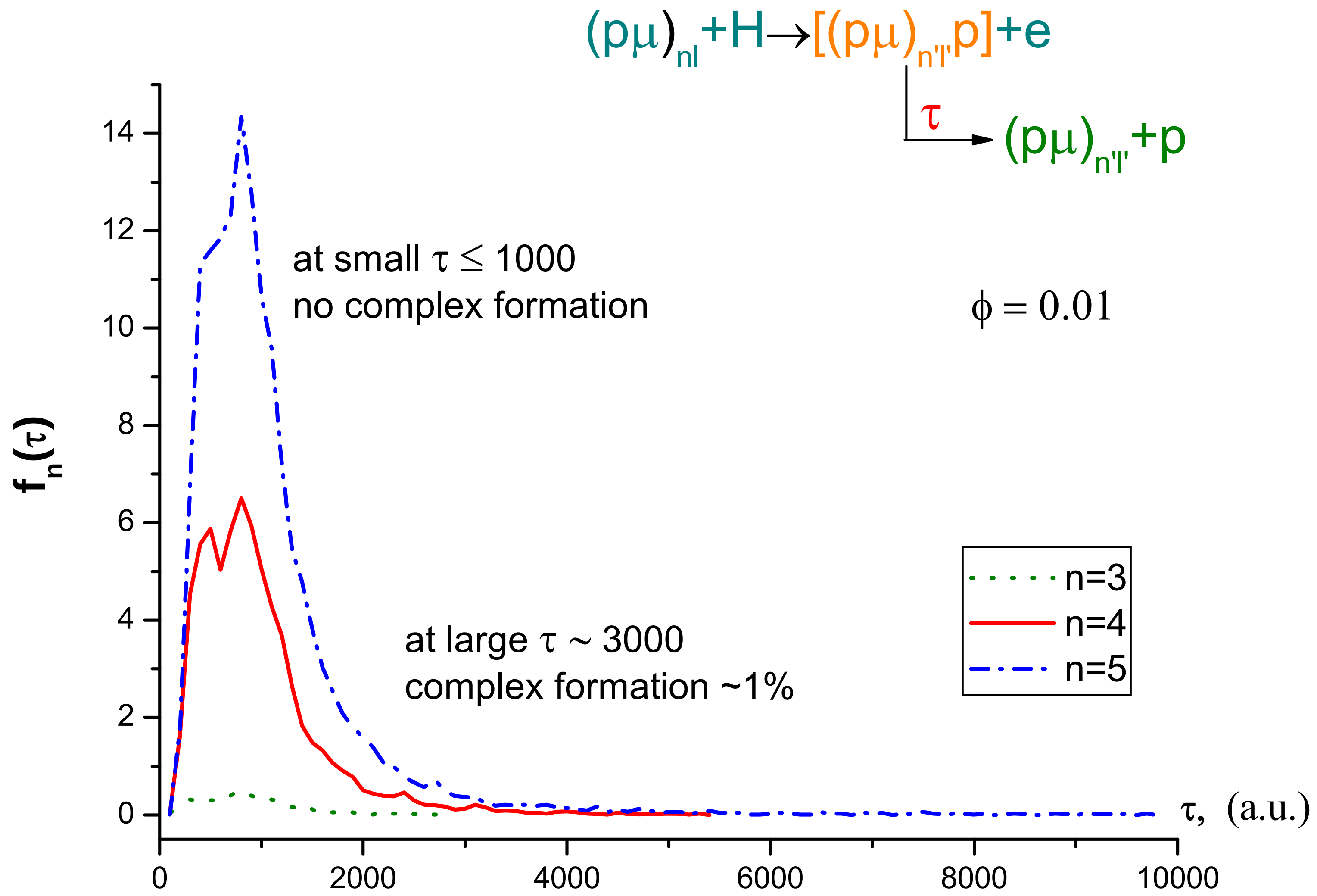
$$\mathrm{W_A} = 1 - \exp(-p_A),$$

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

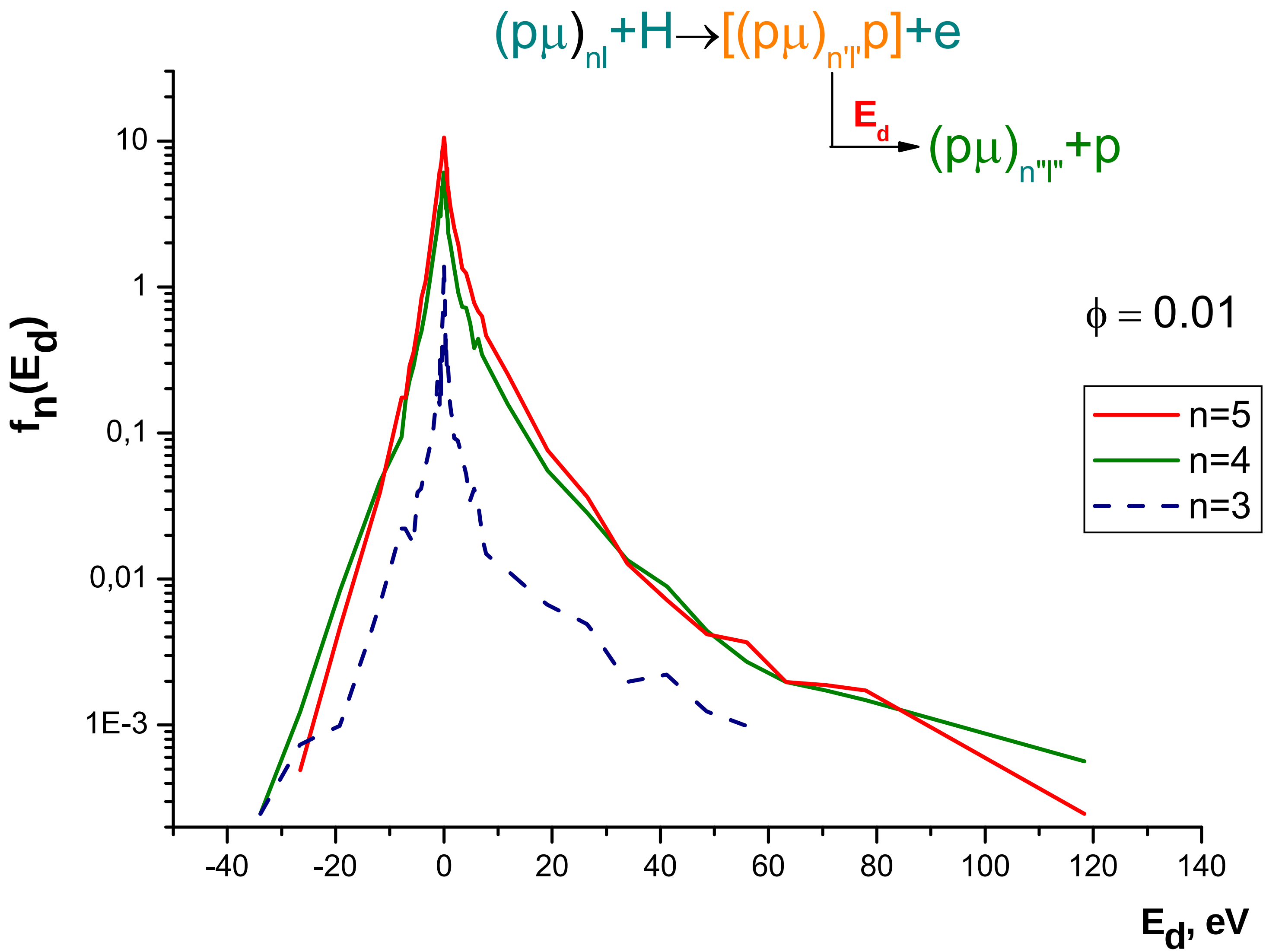
It is necessary to put at the moment $t = t_A$ of the Auger transition:

the screening factor $f(R) = 1, \;\; n' = n - 1, \;\; l' = l - 1.$

The condition $\mathbf{r_{12} > R_0}$ corresponds to the fact of the $[p_1 \mu p_2]$ molecule decay.

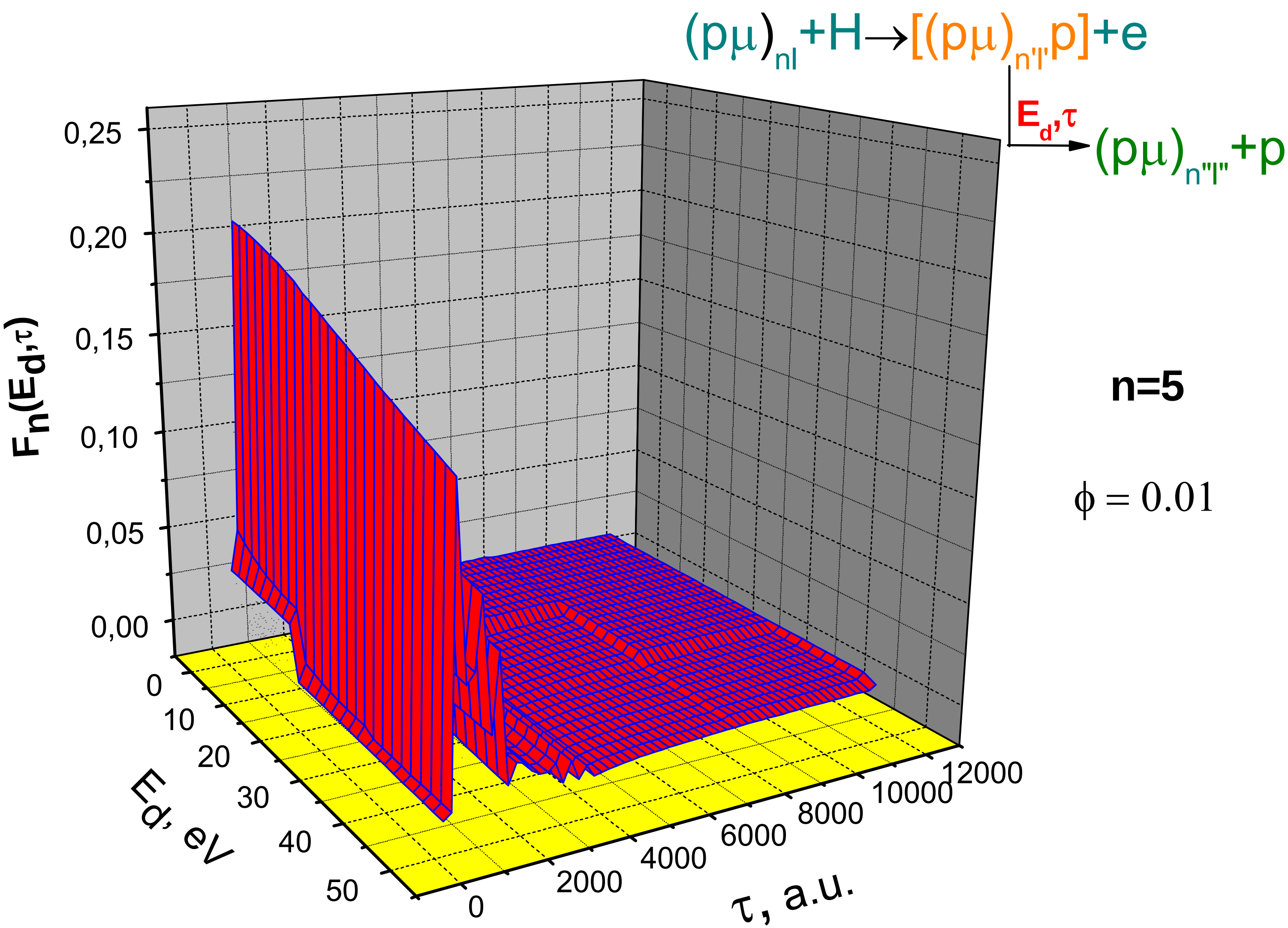


Decay events time distributions of the muonic pμp complexes formed in Auger capture processes.



Distributions of pμ atoms over kinetic energy differences

$E_d = E_{p\mu(nl)} - E_{p\mu(n'l')}$ gained after Auger process.

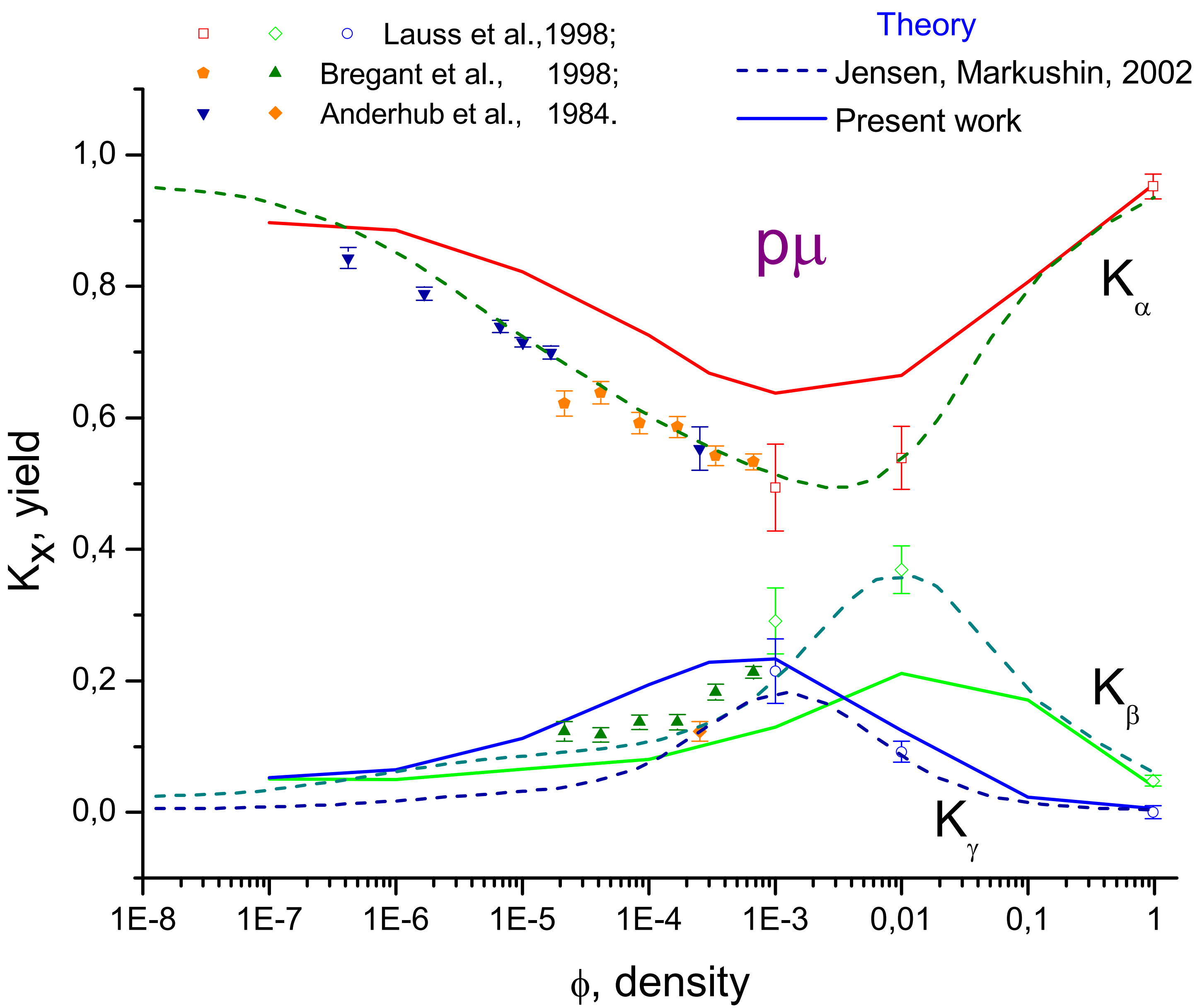


Distribution of muonic complexes pμp decay events over times τ and differences of kinetic energy E_d of pμ atoms :

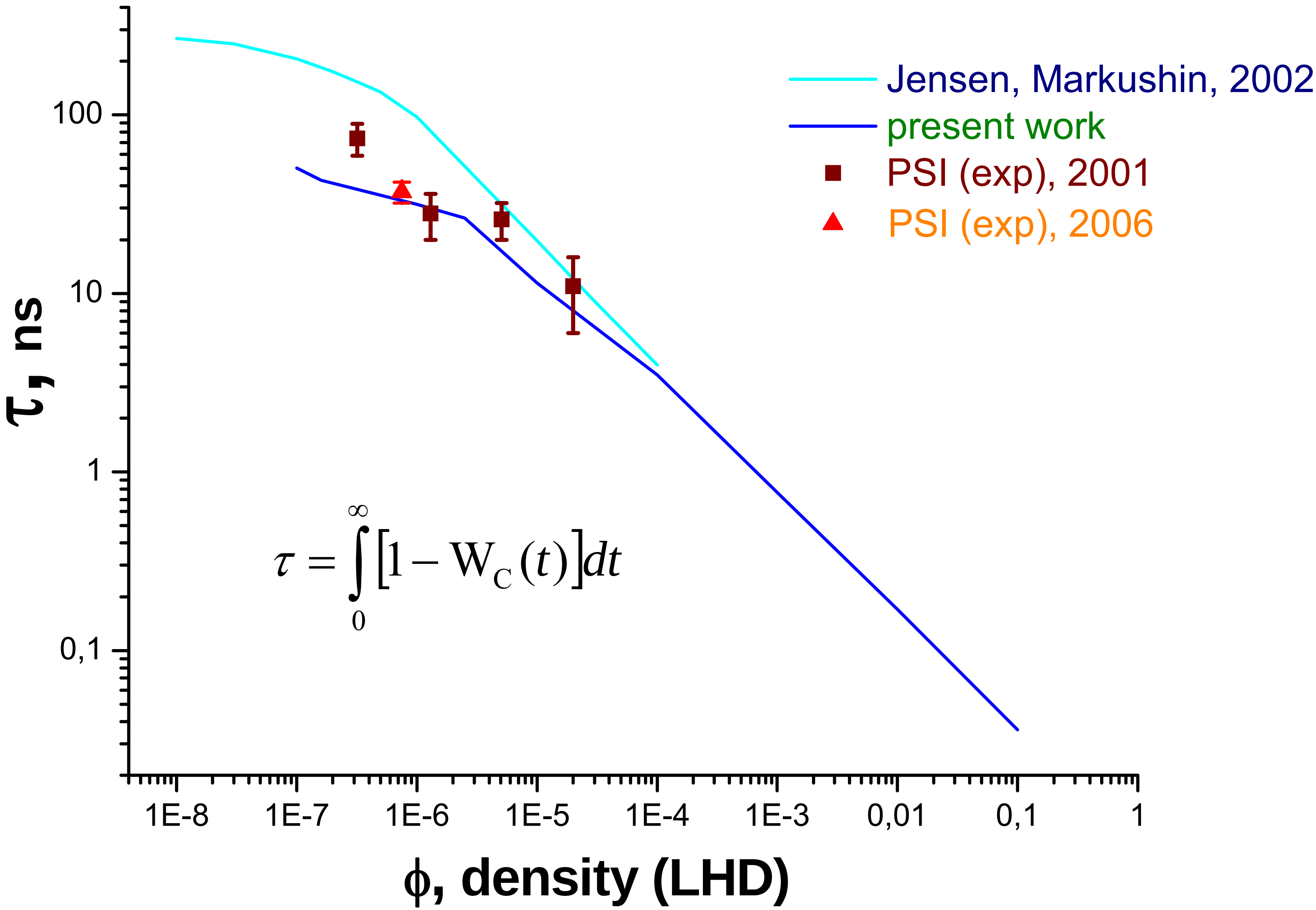
small τ, large E_d – Coulomb transitions;

large τ and E_d – predissociation (~1% of events)

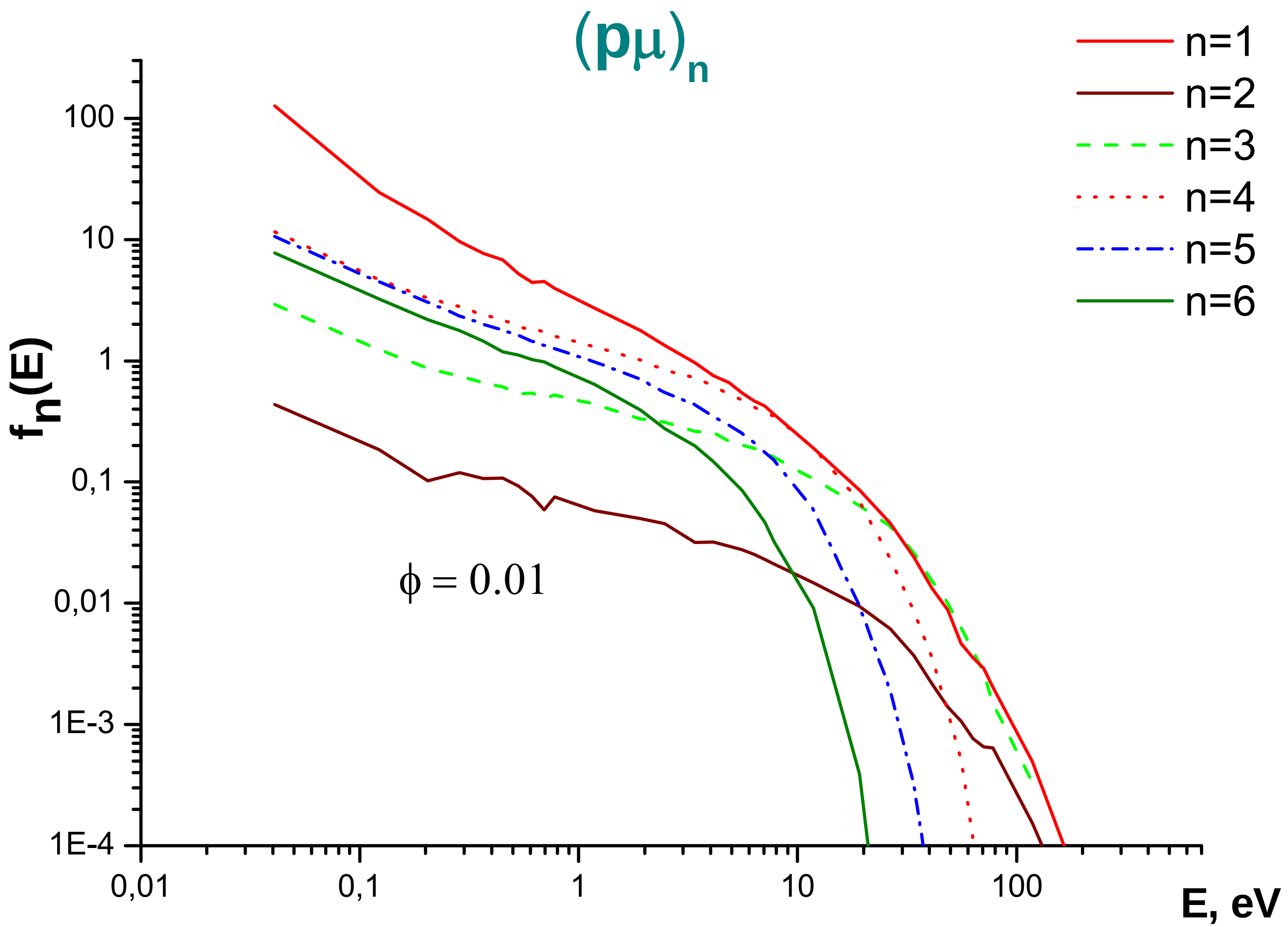
X-ray yields in the muonic hydrogen



pμ atomic cascade time

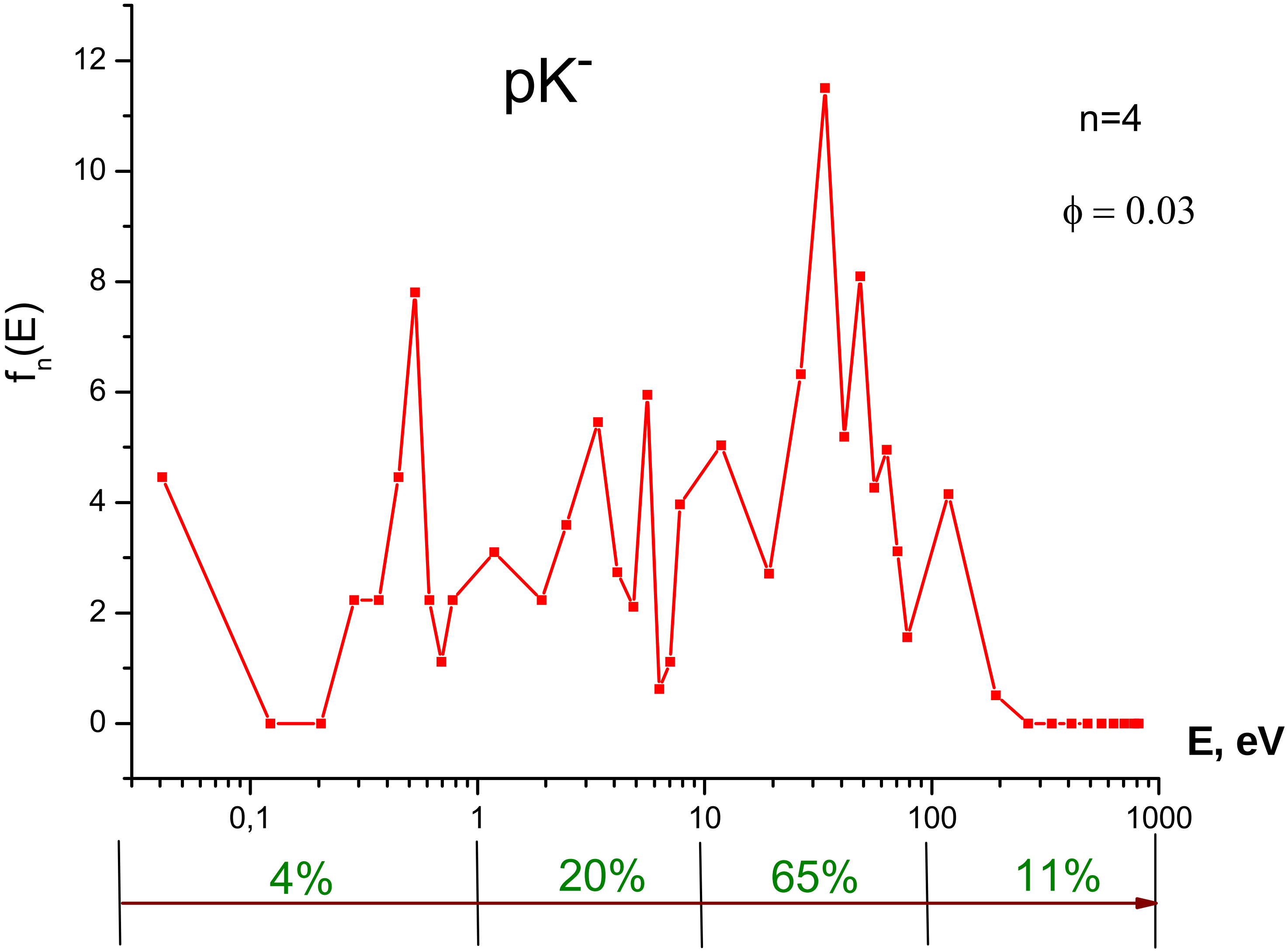


$$\tau = \int_0^\infty \left[1 - W_C(t)\right] dt$$

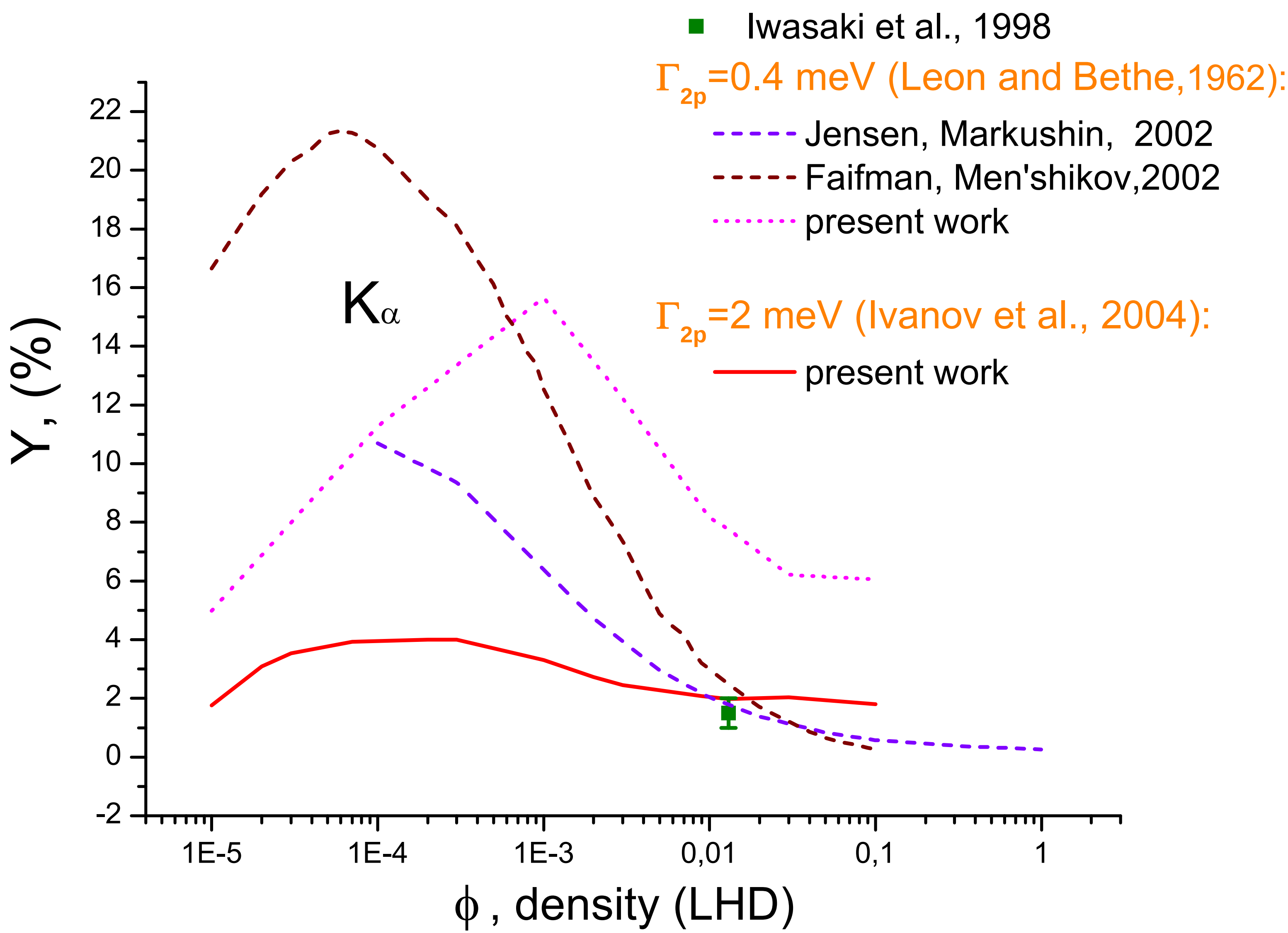


Kinetic energy distributions of (pμ) atoms in *n*-state at density ϕ=0.01 LHD.

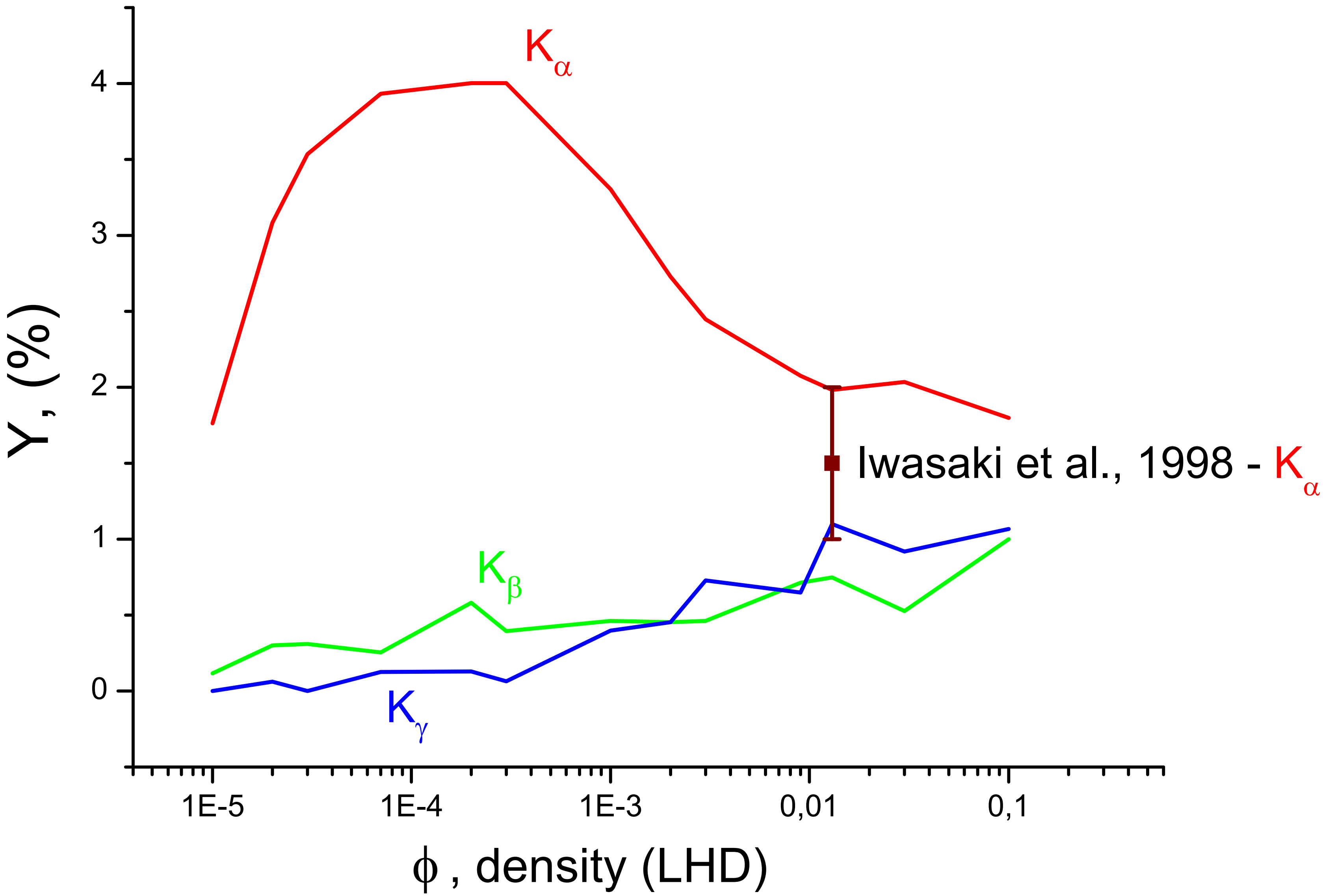
Fractions of pK^- atoms in the different energy intervals



K_α yield of X-rays in pK^- atoms at Γ_{2p}=0.4 meV and Γ_{2p}=2 meV



X-ray yields of kaonic hydrogen atoms



Summary

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

❖ This code does not use any fit parameters, and seems to be more accurate than the calculation scheme requiring a sewing procedure.

❖ The analysis of the kinetics of cascade processes in muonic and kaonic hydrogen atoms leads to conclusion, which is important for simplifying the cascade calculations:

Auger acceleration is negligible for all exotic hydrogen atoms.

❖ The obtained results have demonstrated good agreement between theory and experiment.

❖ The developed code enables to carry out calculations (with sufficient accuracy ~ 20% 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.**