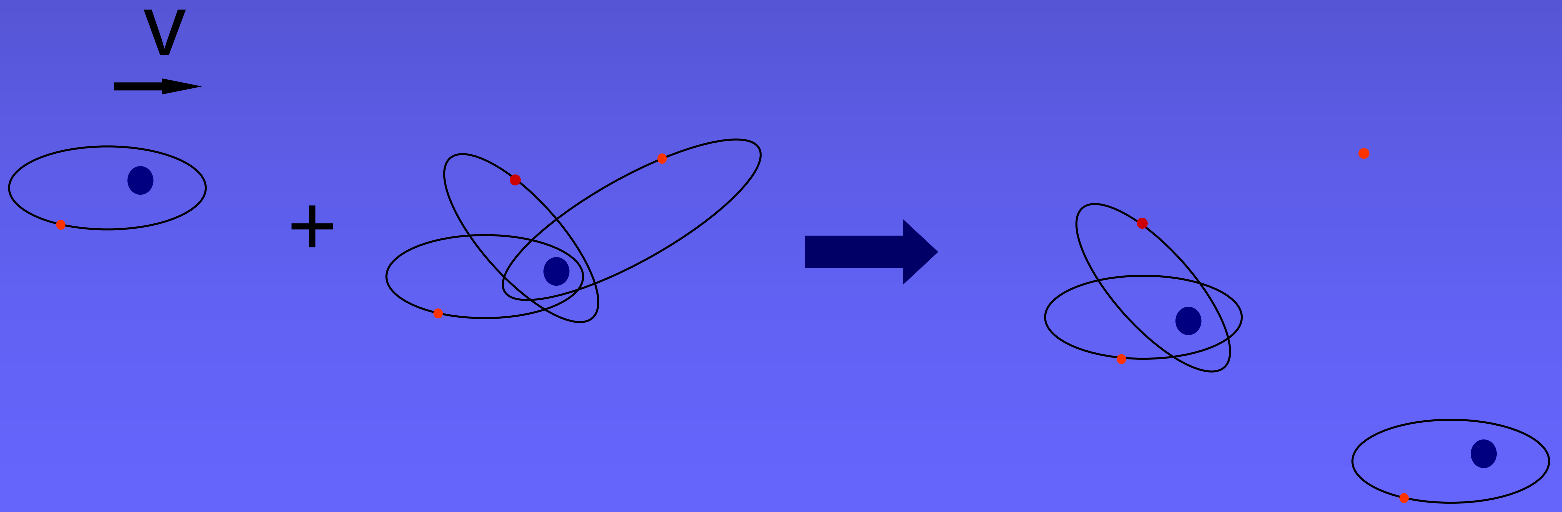
Cross-section modelling for Beam Emission Spectroscopy – Classical treatment

KárolyTőkési[1], Gergő Pokol[2], Örs Asztalos[2], Borbála Szondy[2]

[1]Institute for Nuclear Research, Hungarian Academy of Sciences, Debrecen, Hungary

[2]Institute of Nuclear Techniques, Budapest University of Technology and Economics, Budapest, Hungary



Outlook

- Basic idea
- Classical methods
  CTMC
  - a method of the analysis
- Ionization
- State Selective Capture
- State selective excitation
- Summary

Why?

- Basic research - fundamental physics

- For designing new experiments, such as production of runaway electrons…...

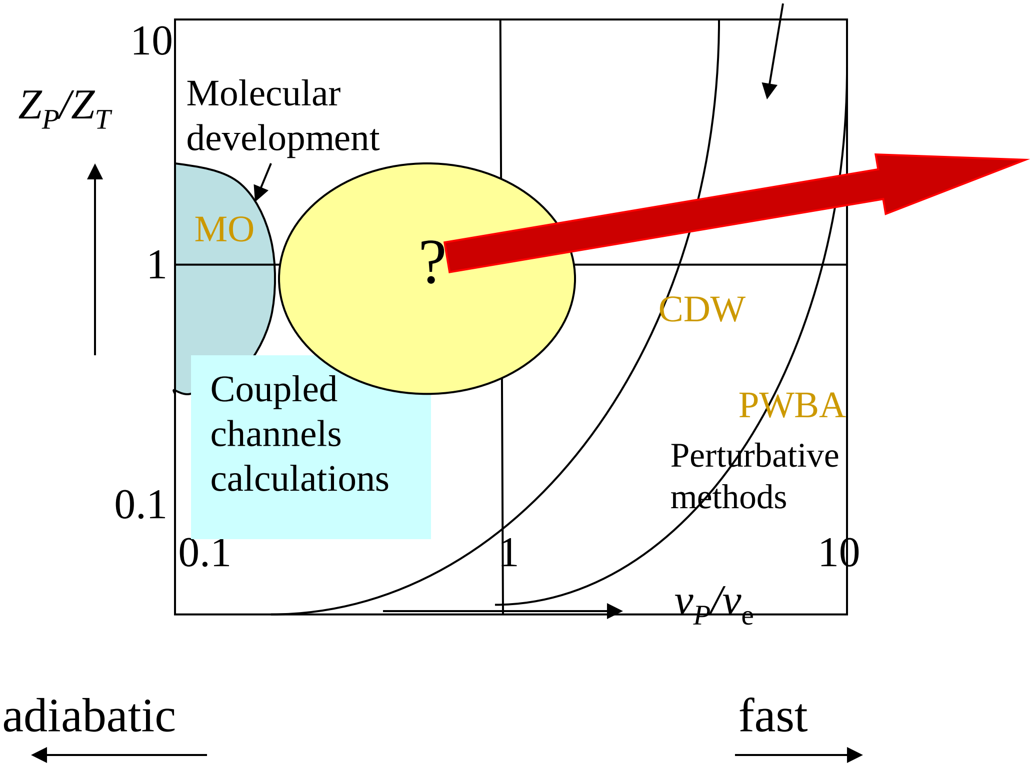
- Technological importance

plasma physics
fusion
analytical methods – medical application

Ionization in ion-atom collisions

Description:

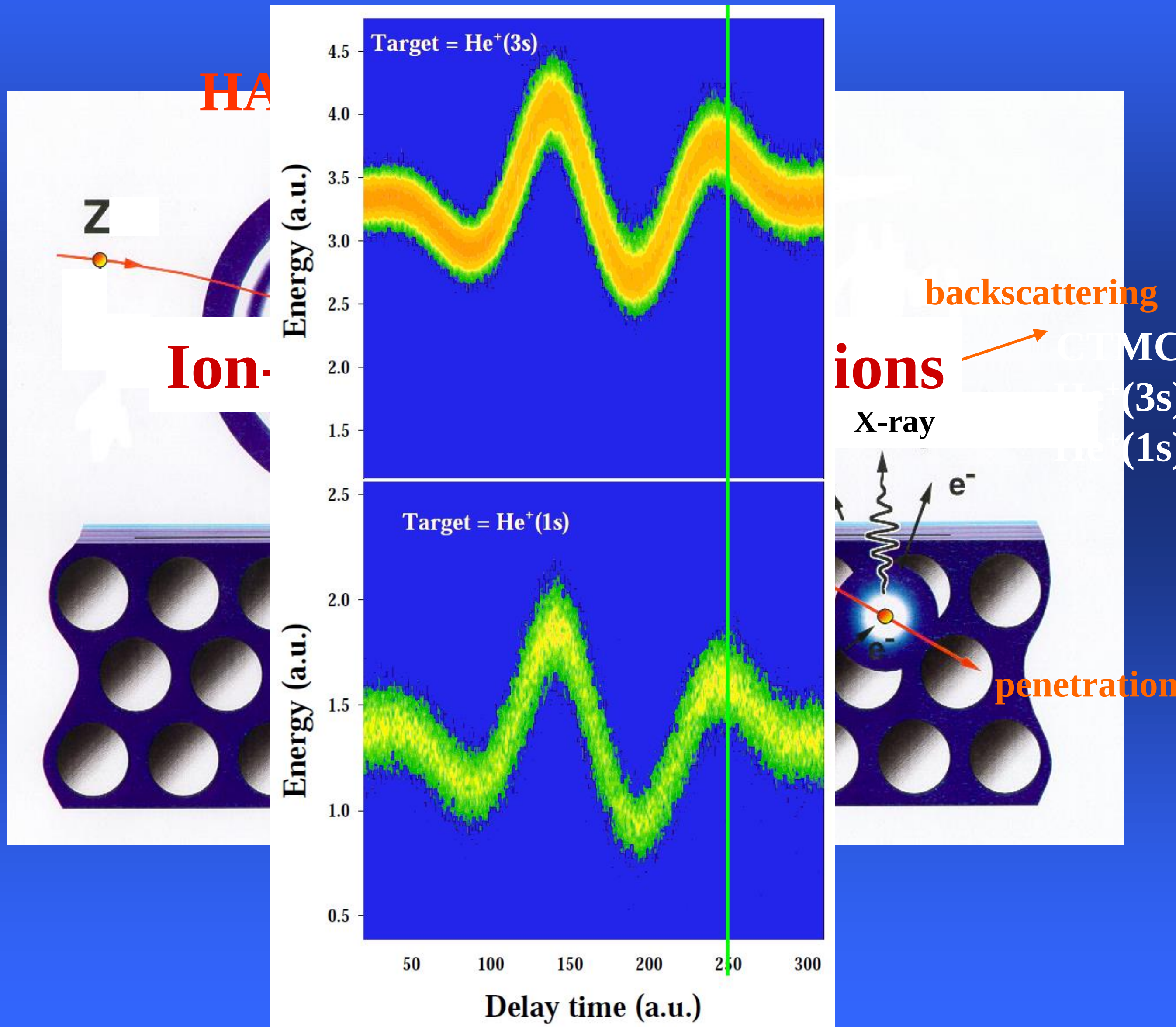
Distorted wawe approximations



Non-perturbative models:

Classical Trajectory Monte Carlo (CTMC) method

Extended applications

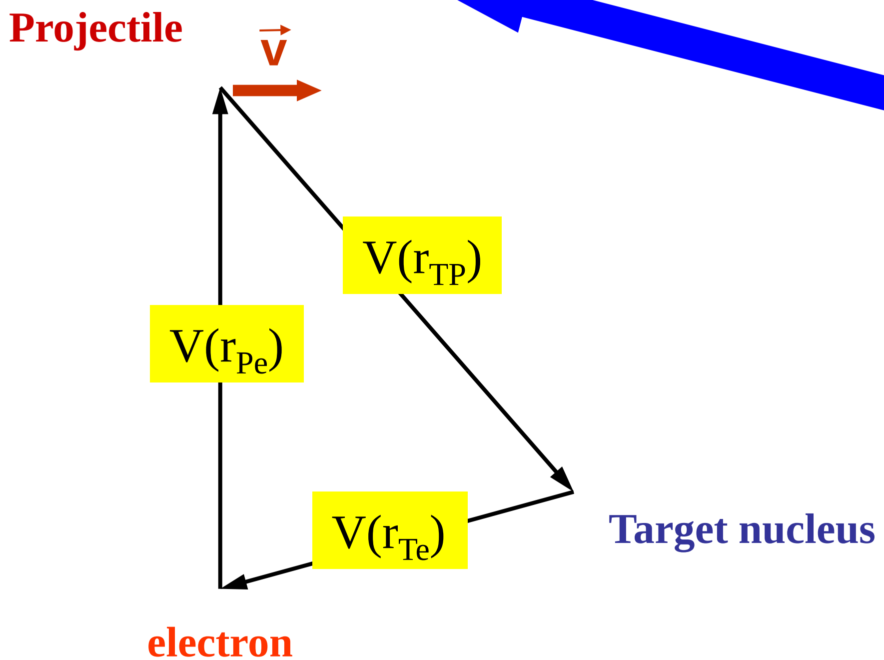


3-body CTMC approach

- **Classical nonperturbative method – „theoretical experiment”**
- **Treats the many-body interactions**

Model potential:

$$V(\mathrm{r}) = -\frac{(Z-1)\Omega(r)+1}{\mathrm{r}}, \quad \text{where} \quad \Omega(\mathrm{r}) = \left[Hd(e^{r/d}-1)+1\right]^{-1}$$



Specific for the present work:
-Screened core potentials for both partners (analytic GSZ model pot.)

-Strategies for extracting the relevant information

- a three-body balance is bound by E and **p** conservation;
- final-state kinematics does not provide information about the mechanism

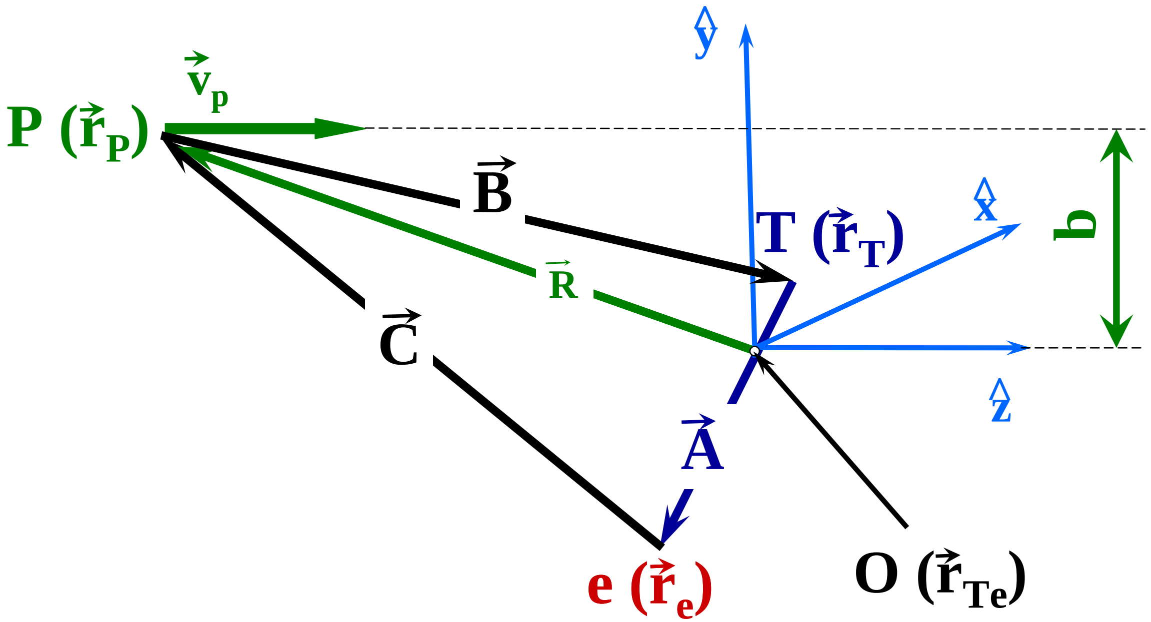


Fig. 1. The relative position vectors of the particles involved in 3-body collisions. $A = \vec{r}_e - \vec{r}_T$, $B = \vec{r}_T - \vec{r}_P$, $\vec{C} = \vec{r}_P - \vec{r}_e$, $\vec{r}_{Te}$ is the position vector of the centre-of-mass of the target system, and b is the impact parameter.

$$L = L_K - L_V$$

$$L_K = \frac{1}{2} m_P \dot{\vec{r}}_P^{\,2} + \frac{1}{2} m_e \dot{\vec{r}}_e^{\,2} + \frac{1}{2} m_T \dot{\vec{r}}_T^{\,2}$$

$$L_V = \frac{Z_P(|\vec{r}_P - \vec{r}_e|) Z_e}{|\vec{r}_P - \vec{r}_e|} + \frac{Z_P(|\vec{r}_P - \vec{r}_T|) Z_T(|\vec{r}_P - \vec{r}_T|)}{|\vec{r}_P - \vec{r}_T|} + \frac{Z_e Z_T(|\vec{r}_e - \vec{r}_T|)}{|\vec{r}_e - \vec{r}_T|}$$

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i}, \qquad \text{(i=P,e,T)}$$

Introducing the relative position vectors $\vec{A} = \vec{r}_e - \vec{r}_T$, $\vec{B} = \vec{r}_T - \vec{r}_P$, and $\vec{C} = \vec{r}_P - \vec{r}_e$, in such a way that $\vec{A} + \vec{B} + \vec{C} = \vec{0}$, we can write

$$m_P \ddot{\vec{r}}_P = -\frac{1}{B^2} f(B, Z_T, Z_P)\,\vec{B} + \frac{Z_e}{C^2}\left(\frac{Z_P(C)}{C} - \frac{\partial Z_P(C)}{\partial C}\right)\vec{C}$$

$$m_e \ddot{\vec{r}}_e = \frac{Z_e}{A^2}\left(\frac{Z_T(A)}{A} - \frac{\partial Z_T(A)}{\partial A}\right)\vec{A} - \frac{Z_e}{C^2}\left(\frac{Z_P(C)}{C} - \frac{\partial Z_P(C)}{\partial C}\right)\vec{C}$$

$$m_T \ddot{\vec{r}}_T = -\frac{Z_e}{A^2}\left(\frac{Z_T(A)}{A} - \frac{\partial Z_T(A)}{\partial A}\right)\vec{A} + \frac{1}{B^2} f(B, Z_T, Z_P)\,\vec{B}$$

$$f(B, Z_T, Z_P) = \frac{Z_P(B)\,Z_T(B)}{B} - Z_P(B)\frac{\partial Z_T(B)}{\partial B} - Z_T(B)\frac{\partial Z_P(B)}{\partial B},$$

$$Z_T(r) = Z_T - (N_T - 1)\left[1 - \frac{1}{\Omega_T(r)}\right]$$

$$\Omega_T(r) = \frac{\eta_T}{\xi_T}(e^{r\xi_T} - 1) + 1$$

$$\frac{\partial Z_T(r)}{\partial r} = \frac{(1 - N_T)\eta_T e^{r\xi_T}}{\Omega_T^2(r)}$$

$$\eta_T = \eta_T^{(0)} + \eta_T^{(1)}(Z_T - N_T)$$

$$\xi_T = \xi_T^{(0)} + \xi_T^{(1)}(Z_T - N_T)$$

$$Z_P(r) = Z_P - N_P\left[1 - \frac{1}{\Omega_P(r)}\right]$$

$$\Omega_P(r) = \frac{\eta_P}{\xi_P}(e^{r\xi_P} - 1) + 1$$

$$\frac{\partial Z_P(r)}{\partial r} = -\frac{N_P\,\eta_P\,e^{r\xi_P}}{\Omega_P^2(r)}$$

$$\eta_P = \eta_P^{(0)} + \eta_P^{(1)}(Z_P - N_P - 1)$$

$$\xi_P = \xi_P^{(0)} + \xi_P^{(1)}(Z_P - N_P - 1)$$

$$\ddot{\vec{A}} = \left[\left(\frac{1}{m_e}\right)\frac{Z_e}{C^2}\left(\frac{Z_P(C)}{C} - \frac{\partial Z_P(C)}{\partial C}\right) + \left(\frac{1}{m_e} + \frac{1}{m_T}\right)\frac{Z_e}{A^2}\left(\frac{Z_T(A)}{A} - \frac{\partial Z_T(A)}{\partial A}\right)\right]\vec{A} +$$
$$+\left[\left(\frac{1}{m_e}\right)\frac{Z_e}{C^2}\left(\frac{Z_P(C)}{C} - \frac{\partial Z_P(C)}{\partial C}\right) - \left(\frac{1}{m_T}\right)\frac{1}{B^2}f(B, Z_T, Z_P)\right]\vec{B}$$

$$\ddot{\vec{B}} = \left[\left(\frac{1}{m_P}\right)\frac{Z_e}{C^2}\left(\frac{Z_P(C)}{C} - \frac{\partial Z_P(C)}{\partial C}\right) - \left(\frac{1}{m_T}\right)\frac{Z_e}{A^2}\left(\frac{Z_T(A)}{A} - \frac{\partial Z_T(A)}{\partial A}\right)\right]\vec{A} +$$
$$+\left[\left(\frac{1}{m_P}\right)\frac{Z_e}{C^2}\left(\frac{Z_P(C)}{C} - \frac{\partial Z_P(C)}{\partial C}\right) + \left(\frac{1}{m_P} + \frac{1}{m_T}\right)\frac{1}{B^2}f(B, Z_T, Z_P)\right]\vec{B}$$

The initial relative motion is specified by the velocity of the projectile and the distance between the projectile and the atomic centre-of-mass:

$$\vec{R} = \begin{pmatrix} 0 \\ b \\ -\sqrt{R^2 - b^2} \end{pmatrix}$$

$$\dot{\vec{R}} = \begin{pmatrix} 0 \\ 0 \\ v_p \end{pmatrix}.$$

A microcanonical ensemble characterizes the initial state of the target constrained to an initial binding energy of the given shell:

$$\rho_{E_0}(\vec{A}, \dot{\vec{A}}) = K_1 \delta(E_0 - E) = \delta\left(E_0 - \frac{1}{2}\mu_{Te}\dot{\vec{A}}^2 - V(A) \right)$$

$$\frac{1}{2}\mu_{Te}\dot{\vec{A}} = E_0 - V(A) > 0$$

$$\rho_{E_0}(E_0, w, \vartheta_r, \vartheta_v, \varphi_r, \varphi_v) = K_1(E_0 - E) \qquad w(A) = \int_0^A d\kappa \mu_{Te} \kappa^2 \sqrt{2\mu_{Te}[E_0 - V(\kappa)]} \qquad 0 < w < w(A_0)$$

$$0 \le w \le w(A_0), \quad 0 \le \varphi_r \le 2\pi, \quad 0 \le \varphi_v \le 2\pi, \quad -1 \le \vartheta_r \le 1, \quad -1 \le \vartheta_v \le 1$$

$$\vec{A} = \begin{pmatrix} A\sqrt{1-\vartheta_r^2}\cos\varphi_r \\ A\sqrt{1-\vartheta_r^2}\sin\varphi_r \\ A\vartheta_r \end{pmatrix}$$

$$\dot{\vec{A}} = \begin{pmatrix} 2/\mu_{Te}\sqrt{E_0 - V(A)}\sqrt{1-\vartheta_v^2}\cos\varphi_v \\ 2/\mu_{Te}\sqrt{E_0 - V(A)}\sqrt{1-\vartheta_v^2}\sin\varphi_v \\ 2/\mu_{Te}\sqrt{E_0 - V(A)}\ \vartheta_v \end{pmatrix}$$

The total and double differential cross-sections were computed with the following formulas:

$$\sigma = \frac{2\pi b_{\max}}{T_N}\sum_j b_j^{(i)}$$

$$\frac{d^2\sigma}{dE d\Omega} = \frac{2\pi b_{\max}}{T_N \Delta E \Delta\Omega}\sum_j b_j^{(i)}$$

The statistical uncertainty of the cross section is given by

$$\Delta\sigma = \sigma\left(\frac{T_N - T_N^{(i)}}{T_N T_N^{(i)}}\right)^{1/2}$$

Exist test in 3-body CTMC simulation

	Direct process	Ionization	Charge transfer
E_{Te}	**<0**	**>0**	**>0**
E_{Pe}	**>0**	**>0**	**<0**

$$\ddot{\vec{A}} = \left[\frac{(N_2 + N_3)Z_2 Z_3}{\left|\vec{A}\right|^3} + \frac{N_2 Z_1 Z_2}{\left|\vec{A}+\vec{B}\right|^3} \right] \vec{A} + \left[\frac{N_2 Z_1 Z_2}{\left|\vec{A}+\vec{B}\right|^3} - \frac{N_3 Z_1 Z_3}{\left|\vec{B}\right|^3} \right] \vec{B}$$

$$\ddot{\vec{B}} = \left[-\frac{N_3 Z_2 Z_3}{\left|\vec{A}\right|^3} + \frac{N_1 Z_1 Z_2}{\left|\vec{A}+\vec{B}\right|^3} \right] \vec{A} + \left[\frac{N_1 Z_1 Z_2}{\left|\vec{A}+\vec{B}\right|^3} + \frac{(N_1 + N_3)Z_1 Z_3}{\left|\vec{B}\right|^3} \right] \vec{B}$$

Classical principal quantum number:

$$n_c = Z\sqrt{\frac{\mu}{2U}}$$

n_c is "quantized" to a specific n [J.Phys.B**17** (1987) 3923]:

$$\left[(n-1)(n-0.5)n\right]^{1/3} \leq n_c \leq \left[n(n+0.5)(n+1)\right]^{1/3}$$

Classical orbital angular momentum:

$$l_c = \left[(x\dot{y} - y\dot{x})^2 + (x\dot{z} - z\dot{x})^2 + (y\dot{z} - z\dot{y})^2\right]^{1/2}$$

l_c is "quantized" to a specific l:

$$l \leq l_c \frac{n}{n_c} \leq l + 1$$

Cross section:

$$\sigma_{(n,l)} \frac{2\pi b_{\max} \sum_j b_j^{(n,l)}}{N}$$

Quasi Classical Trajectory
Monte Carlo method

Heisenberg potential

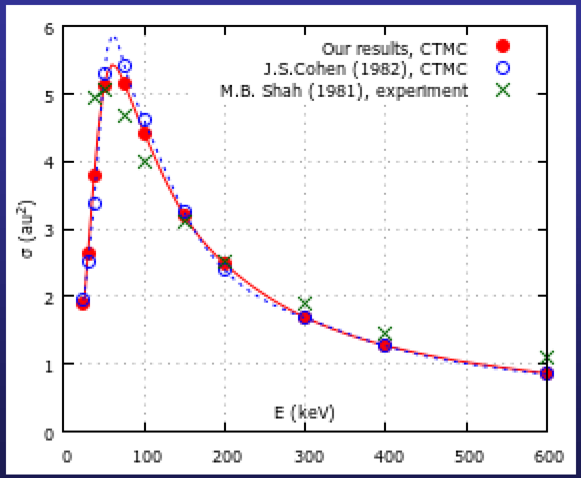
$$V_H(r_i, p_i) = \frac{(\xi_H \hbar)^2}{4\,\alpha\,\mu\, r_i^2} \exp\left(\alpha\left[1 - \left(\frac{r_i p_i}{\xi_H \hbar}\right)^4\right]\right).$$

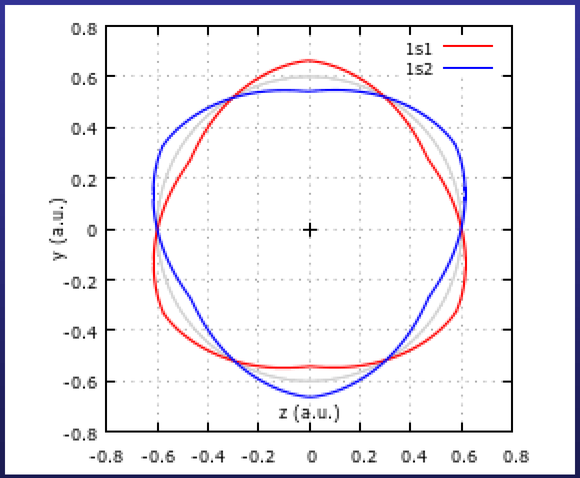
Pauli potential

$$V_P(r_i, p_{ij}) = \frac{(\xi_P \hbar)^2}{4\,\alpha\, m_e\, r_{ij}^2} \exp\left(\alpha\left[1 - \left(\frac{r_{ij} p_{ij}}{\xi_P \hbar}\right)^4\right]\right).$$

$$H_{KW} = H_0 + \sum_i \left[V_H(r_i, p_i) + \sum_{j > i} \delta_{s_i, s_j} V_P(r_{ij}, p_{ij}) \right],$$

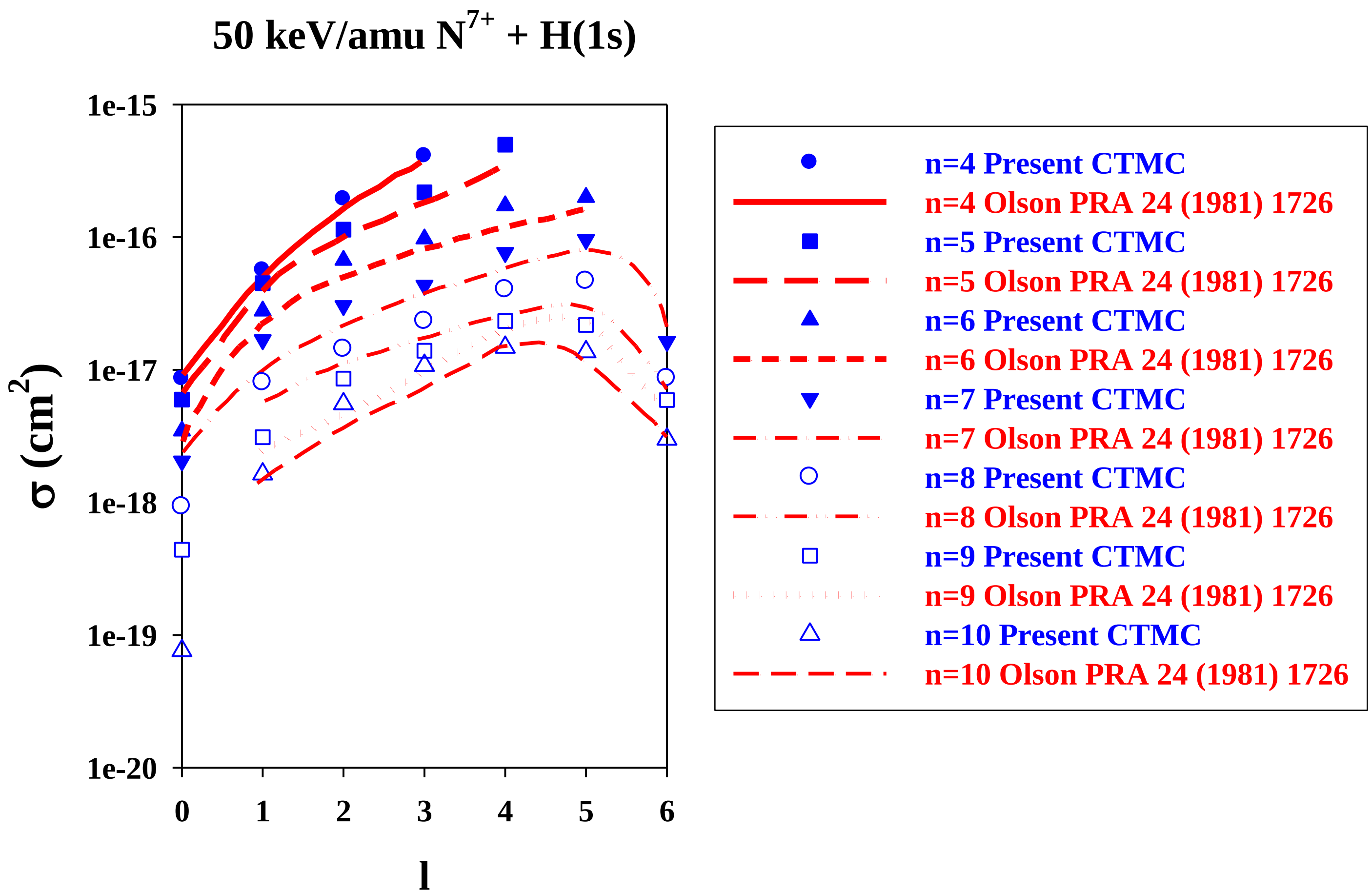
Orbitals of a helium atom represented



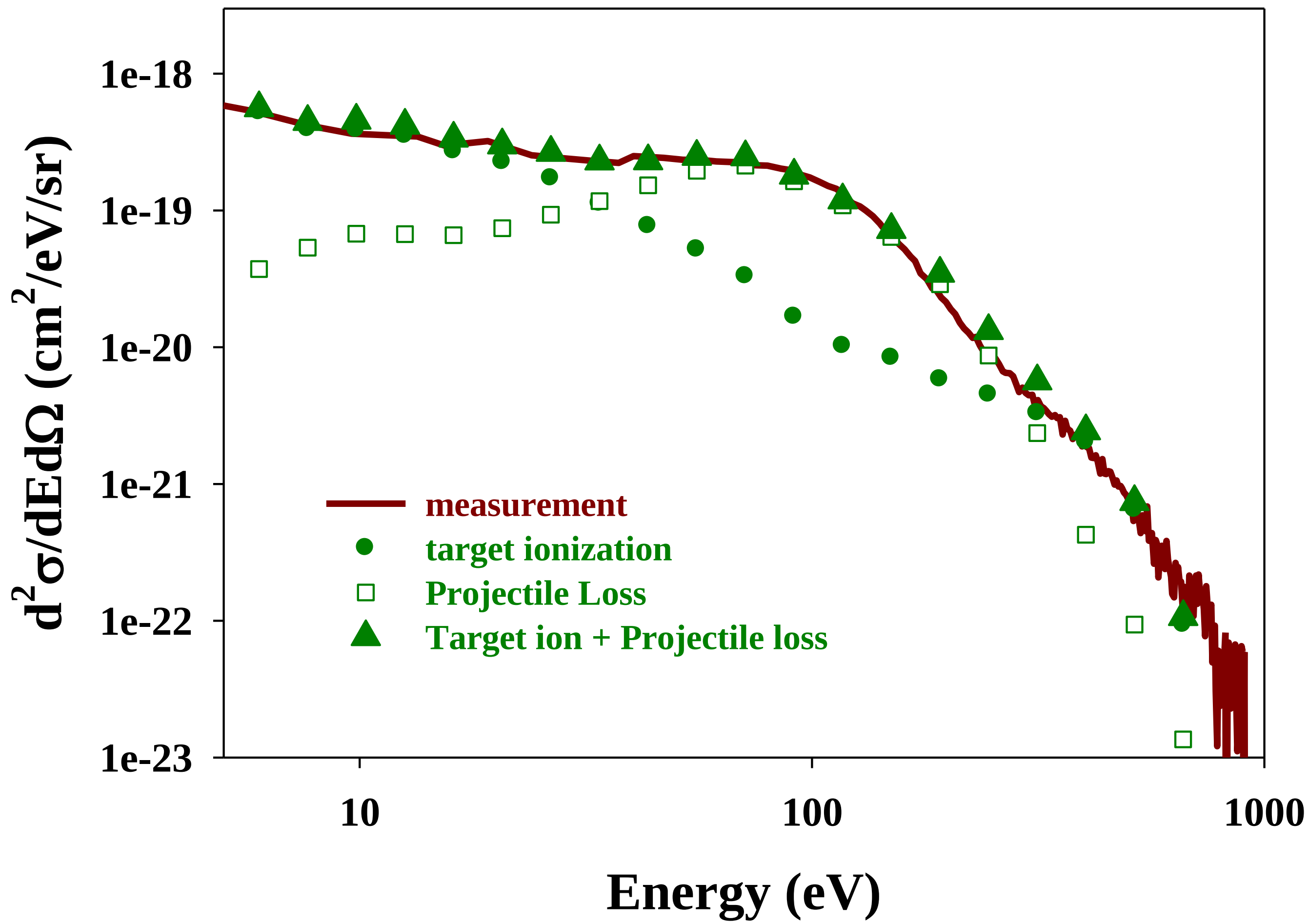


Can it be apply?
What is the accuracy?

State selective capture cross sections



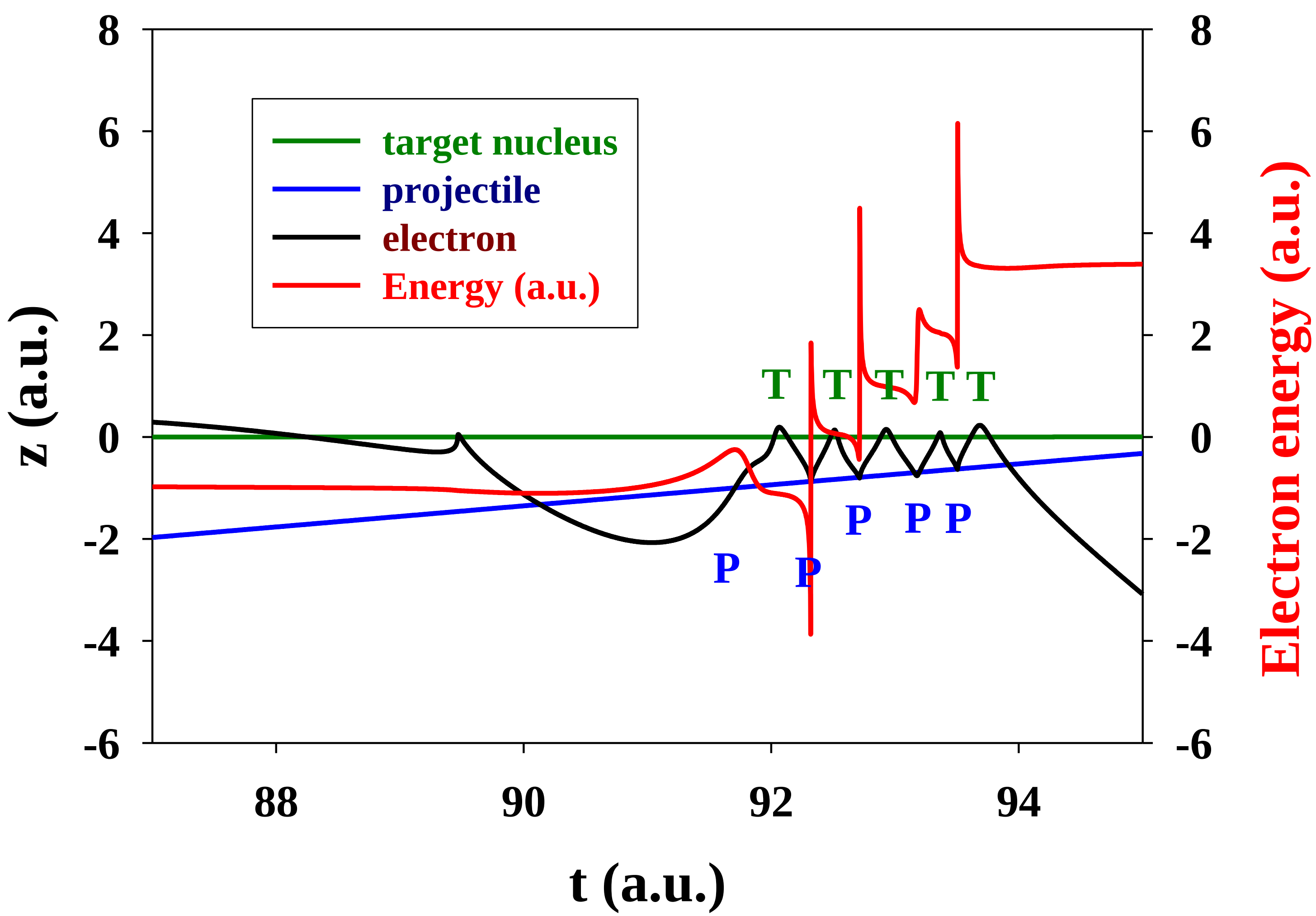
Doubly differential cross sections for ionization of neon by 2.4 MeV C+ ions.
θ= 130°



Visualization

Long ping-pong game (15 keV N^+ + Ar)

P-T-P-T-P-T-P-T-P-T



How many particles can be treat?

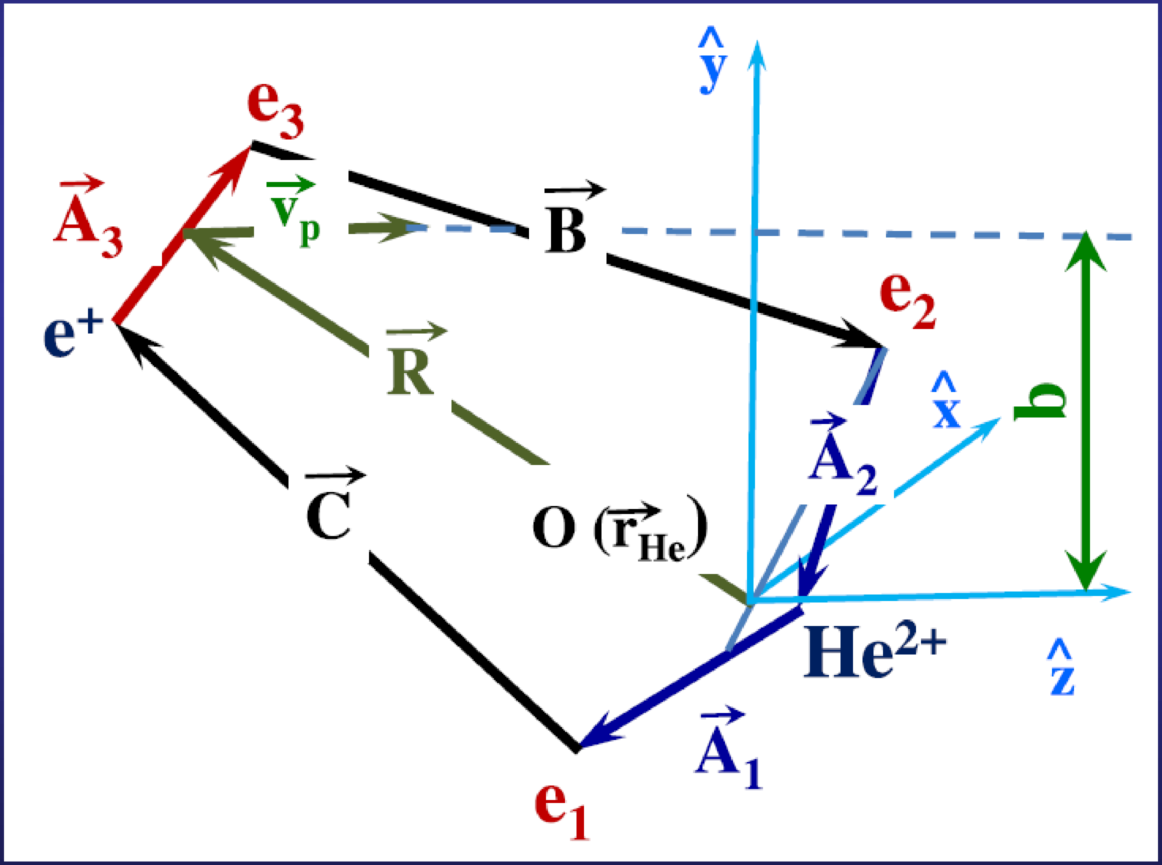
Interaction of positronium with helium atoms – the classical treatment of the 5-body collision system

The relative position vectors of the particles involved in 5-body collisions

E_{ps}=0.25 au.

$E_{He\text{-}1}$=0.903 au.
$E_{He\text{-}2}$=2.0 au.

18 different exit channels



Eur. Phys. J. D (2014) 68: 255

Single electron loss of the target

$$\mathrm{Ps} + \mathrm{He}(1's^2) \rightarrow \mathrm{Ps} + \mathrm{He}^+ + \mathrm{e}^-$$

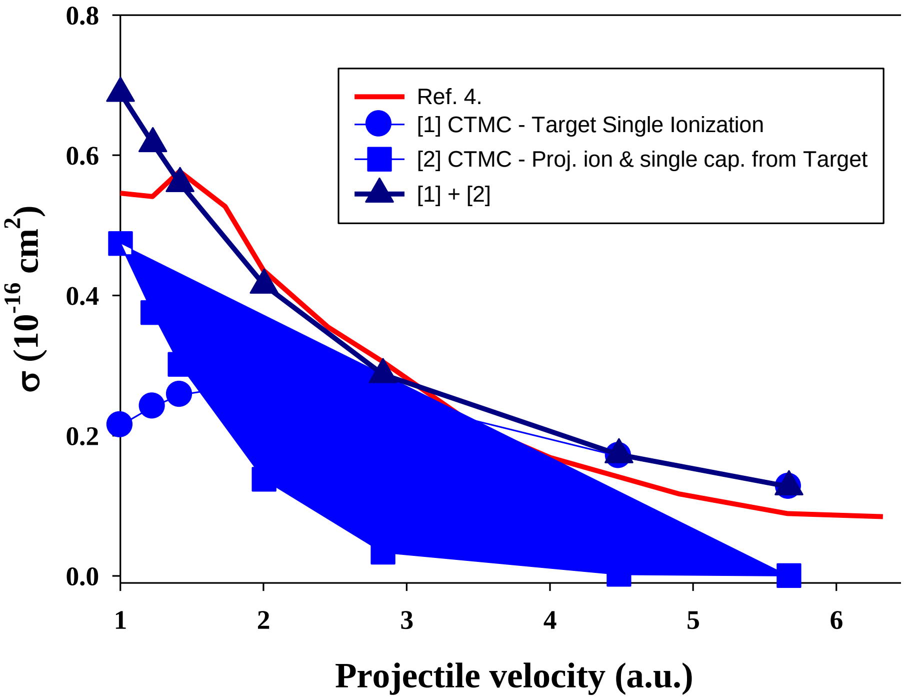
$$(\mathrm{e}^+, \mathrm{e}_3^-) + \mathrm{He}(\mathrm{e}_1^-, \mathrm{e}_2^-) \rightarrow (\mathrm{e}^+, \mathrm{e}_3^-) + \mathrm{He}^+(\mathrm{e}_1^-) + \mathrm{e}_2^-$$

$$(\mathrm{e}^+, \mathrm{e}_3^-) + \mathrm{He}(\mathrm{e}_1^-, \mathrm{e}_2^-) \rightarrow (\mathrm{e}^+, \mathrm{e}_3^-) + \mathrm{He}^+(\mathrm{e}_2^-) + \mathrm{e}_1^-$$

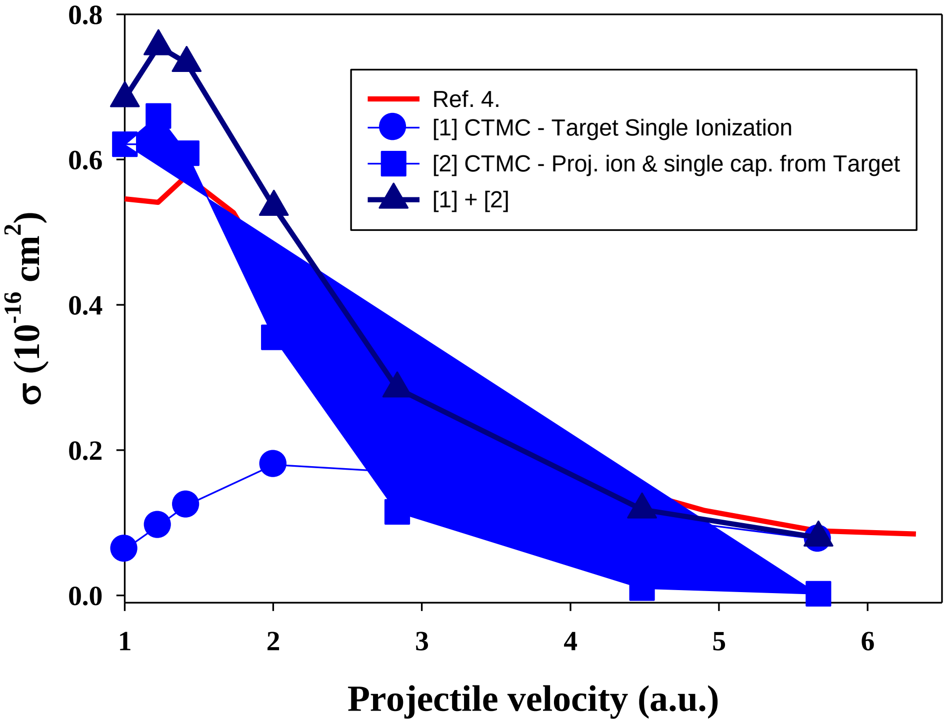
$$(\mathrm{e}^+, \mathrm{e}_3^-) + \mathrm{He}(\mathrm{e}_1^-, \mathrm{e}_2^-) \rightarrow (\mathrm{e}^+, \mathrm{e}_1^-) + \mathrm{He}^+(\mathrm{e}_2^-) + \mathrm{e}_3^-$$

$$(\mathrm{e}^+, \mathrm{e}_3^-) + \mathrm{He}(\mathrm{e}_1^-, \mathrm{e}_2^-) \rightarrow (\mathrm{e}^+, \mathrm{e}_2^-) + \mathrm{He}^+(\mathrm{e}_1^-) + \mathrm{e}_3^-$$

H^0 + He

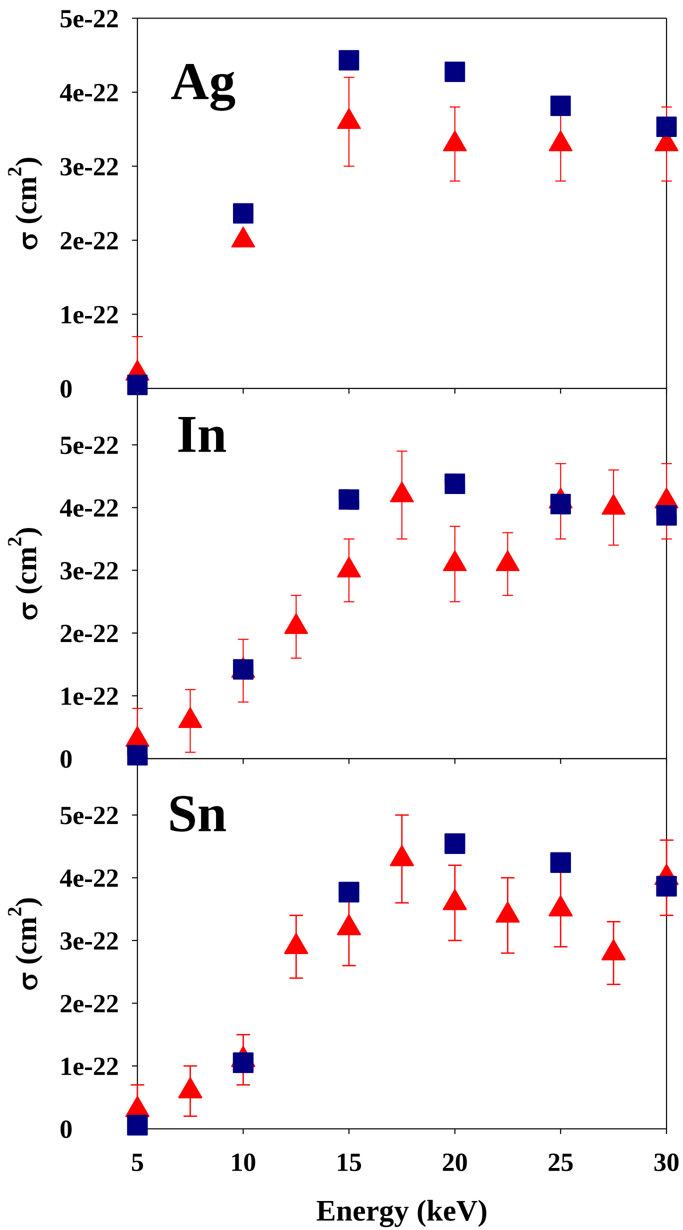


PS + He



L-shell x-ray production cross sections of Ag, In and Sn by positron impact

L-shell x-ray production cross sections of Ag, In and Sn as a function of the positron impact from the threshold energy up to 30 keV. Trinagles: experiment [1], squares: present CTMC results.



In the present cases, a very large number of classical trajectories were computed because the total cross sections decrease dramatically with decreasing incident projectile energies. At low impact energies, 20 million histories were calculated, while at 25 and 30 MeV impact energy, 2 million classical trajectories were evaluated.

[1] Y, Nagashima, W. Shigeta, T. Hyodo, M. Iwaki, 2007 *Radiation Physics and Chemistry* 76 465.

Plan -- Outlook

Classical simulations

in charged particles-atom collsions

- **Ionization**
- **State Selective Exciation**
- **State Selective Charge Transfer**

Attending on

- **Code Comparison Workshop on Electron Dynamics in Atomic Collisions**
- **Code Comparison Workshop on Neutral Beam Beam Penetration and Bea-based Photoemission**

Conclusions

- Classical method (CTMC) reproduce different experiments for collisions between charged particles and atoms,
- gives accurate cross sections for ionization

  Capture

  Excitation
- valid in wide projectile energy range
- can descibe partial cross sections

Thank you!