Total and differential ionization cross sections for antiproton helium collisions

I. F. Barna

Outline

- Motivation, introduction
- The coupled channel method
  wavefunction & spectrum, collision
- Results, total and differential ionization cross sections
- Summary and Outlook

The Hamiltonian of the system

The time-dependent Schrödinger equation:

$$i\frac{\partial}{\partial t}\Psi(\vec{r}_1,\vec{r}_2,t) = (\hat{H}_{He} + \hat{V}(t))\Psi(\vec{r}_1,\vec{r}_2,t)$$

- $\hat{V}(t)$ projectile-electron interaction
- $\Psi(\vec{r}_1,\vec{r}_2,t)$ CI. wave function of helium

The unperturbed helium Hamiltonian

$$\hat{H}(\vec{r}_1,\vec{r}_2)_{He} = -\frac{\vec{\nabla}_1^2}{2} - \frac{\vec{\nabla}_2^2}{2} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{|\vec{r}_1 - \vec{r}_2|}$$

- spin-spin, spin-orbit, and mass polarisation terms are neglected

The coupled-channel equation

Ansatz:

$$\Psi(\vec{r}_1, \vec{r}_2, t) = \sum_{j=1}^{N} a_j(t)\Phi_j(\vec{r}_1, \vec{r}_2)e^{-iE_j t}$$

Leads to a system of first-order-differential equations for the coefficients a_j :

$$\frac{da_k(t)}{dt} = -i\sum_{j=1}^{N} V_{kj}(t)e^{-i(E_j - E_k)t}a_j(t) \quad (k = 1....N)$$

$V_{kj}(t) = \langle \Phi_k | \hat{V}(t) | \Phi_j \rangle$ coupling matrix

Initial conditions:

$$a_k\,(t \to -\infty) = \begin{cases} 1 & k = 1 \\ 0 & k \neq 1 \end{cases}$$

the final probability for each channel:

$$P_k(b, t \to \infty) = \mid a_k(t \to \infty) \mid^2$$

total cross section:

$$\sigma_k = 2\pi \int_0^\infty P_k(b) b db$$

The wavefunction

Configuration interaction(CI) expansion of $\Phi_j(\vec{r}_1, \vec{r}_2)$ in terms of two-particle basis functions f_μ

$$\Phi_j(\vec{r}_1, \vec{r}_2) = \sum_\mu b_\mu^j f_\mu(\vec{r}_1, \vec{r}_2).$$

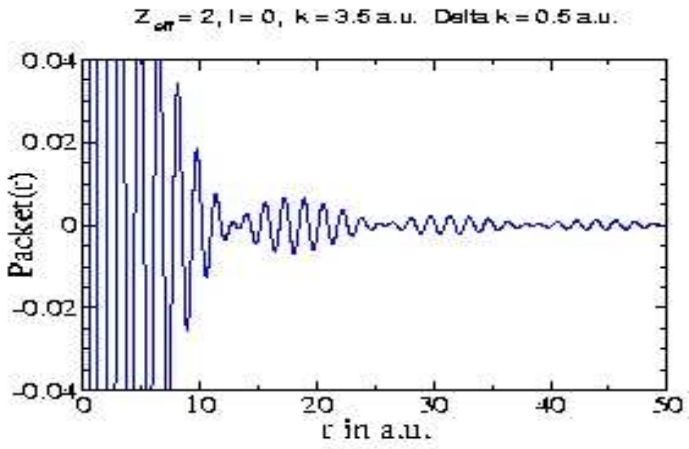
where $f_\mu(\vec{r}_1, \vec{r}_2)$ are symmetric (S=0) products of
1. Slater-type orbitals:

$$\chi_{n,l,m,\kappa}(\vec{r}) = C(n, \kappa) r^{n-1} e^{-\kappa r} Y_{l,m}(\theta, \varphi)$$

2. regular Coulomb wave packets:

$$\varphi_{k,l,m,\tilde{Z}}(\vec{r}) = N(k, \Delta k) \int_k^{k+\Delta k} R_l(\eta, \rho) dk' Y_{l,m}(\theta, \varphi)$$

- $\eta = \tilde{Z}/k'$, $\rho = k'r$, $\tilde{Z}$ effective charge
- $N(k, \Delta k)$, $C(n, \kappa)$ normalisation constants



l= 0, 1, 2
single particle
wavefunctions
coupled to:
L = 0, 1, 2
states

Electron densities

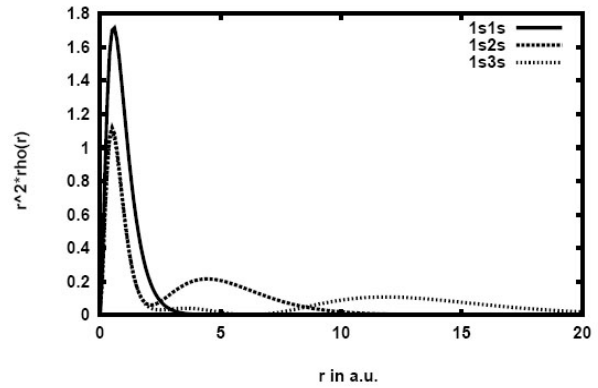


Figure 3.4: Electron density of the ground state and the following two single-excited states.

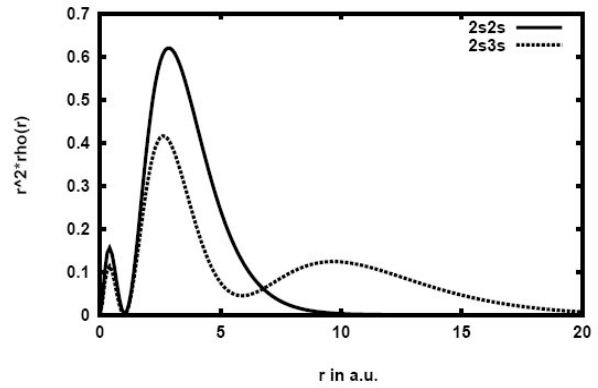


Figure 3.5: Electron densities of double-excited states.

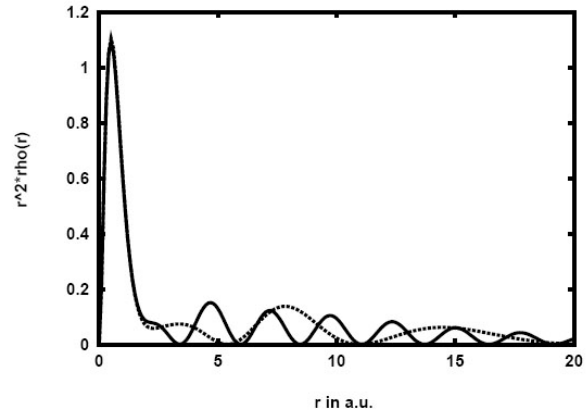


Figure 3.6: Electron densities of single-ionized states, solid line: with packages and dashed line: without packages.

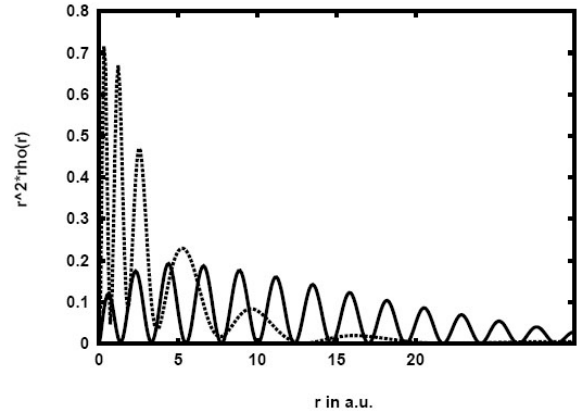
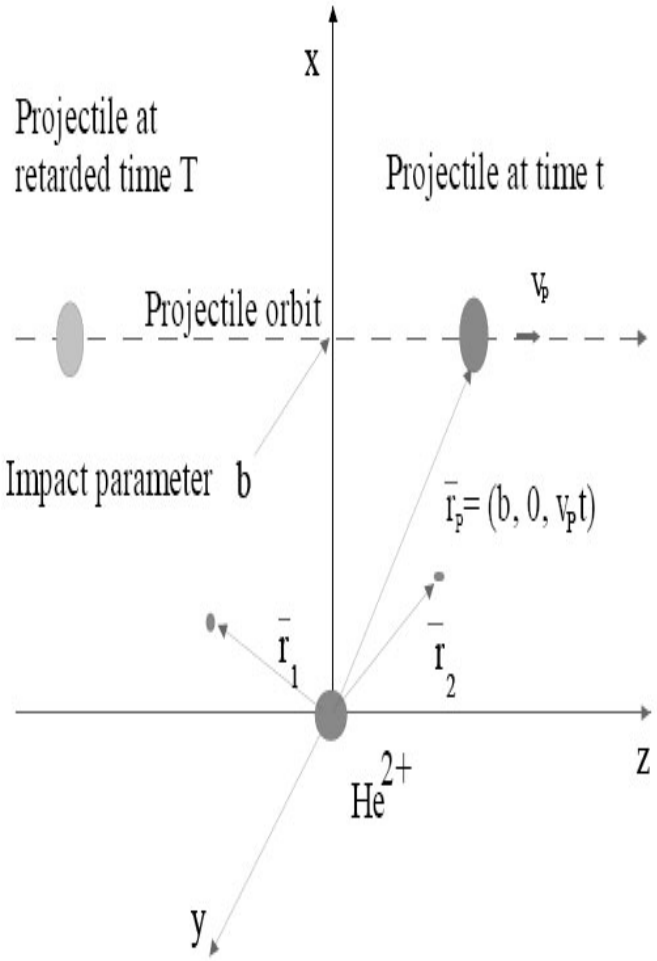


Figure 3.7: Electron densities of double-ionized states, solid line: with packages and dashed line: without packages.

Coordinate system



Semiclassical approximation:
electrons - quantum objects
nucleus & projectile - classical point charges

projectile flies on a straight line (above 10 keV)

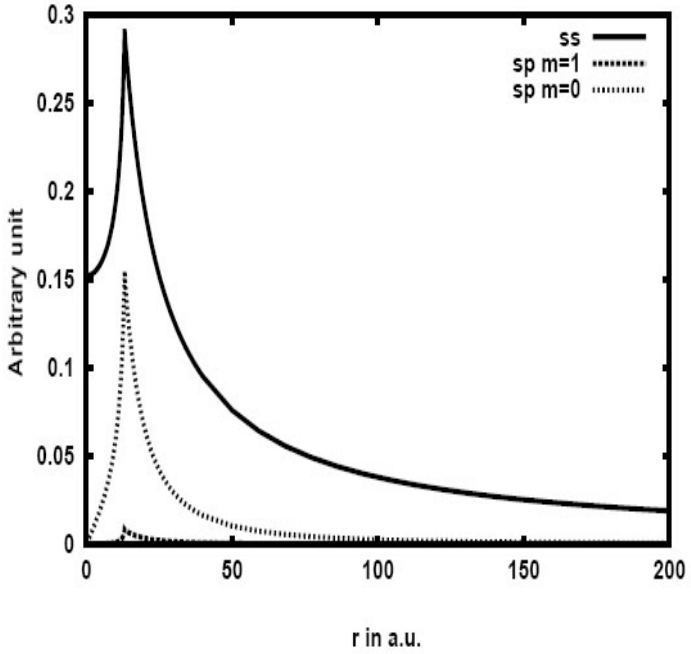
Antiproton Electron Interaction

$$\hat{H}(\vec{r}_1,\vec{r}_2,t) = \frac{(\vec{p}_1+\vec{A}(\vec{r}_1,t))^2}{2} + \frac{(\vec{p}_2+\vec{A}(\vec{r}_2,t))^2}{2} - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}} - \Phi(\vec{r}_1,t) - \Phi(\vec{r}_2,t).$$

- Minimal coupling for the projectile fields
- Lienard-Wiechert reterded potentials for relativistic projectiles
- Simple time-dependent Coulomb scalar potential in this case
- Three dimensional numerical integrals for the matrix elements

→ Symmetries have to be used out,
time reversal,
asimuthal,
and magnetic quantum number

Multipole expansion



- Large number of 3dim. num. integration (b, t dependent)
- the angular part are the same

$$\text{Multipole}(r,\gamma,b,t) = \int_{\Omega} \frac{Y_{l_1,m_1}(\theta,\varphi)^* \cdot Y_{l_2,m_2}(\theta,\varphi)}{R(r,\theta,\varphi,\gamma,b,t)} d\Omega$$

Angular Differential Cross Section

we take the density operator to calculate the electron density after the collision:

$$\rho(\vec{r}) = \left\langle \Psi(\vec{r}_1, \vec{r}_2, t \to \infty) \left| \sum_{i=1,2} \hat{\delta}(\vec{r} - \vec{r}_i) \right| \Psi(\vec{r}_1, \vec{r}_2, t \to \infty) \right\rangle$$

1.) we apply the Fesbach projection to extract the single-ionised contribution from the wave function

$$|\Psi_{ion}\rangle = (1 - \hat{P}_b - \hat{P}_{di})|\Psi(\vec{r}_1, \vec{r}_2, t \to \infty)\rangle$$

2.) integrate the radial and asymuthal angle to get the polar distribution of the ionised electron

$$P(\theta) = \frac{1}{2\pi} \int_0^{\infty} \int_0^{2\pi} \langle \Psi_{ion}| \sum_{i=1,2} \hat{\delta}(\vec{r} - \vec{r}_i)|\Psi_{ion}\rangle r^2 dr d\varphi =$$

$$\frac{1}{\pi} \int_0^{\infty} \int_0^{2\pi} \int_{\vec{r_1}} |\Psi_{ion}(r, \theta, \varphi; \vec{r}_1)|^2 \, d^3 r_1 r^2 dr d\varphi$$

the angular dependence of $P(\theta)$ is given by products of associated Legendre polynomials

Identification of the final states

$$\Phi_j(\mathrm{r}_1,\mathrm{r}_2) = \sum_\lambda \left(C^{\mathrm{bb}}_{\lambda j,LM}\Psi^{\mathrm{bb}}_{\lambda,LM} + C^{\mathrm{bi}}_{\lambda j,LM}\Psi^{\mathrm{bi}}_{\lambda,LM} + C^{\mathrm{ii}}_{\lambda j,LM}\Psi^{\mathrm{ii}}_{\lambda,LM}\right)$$

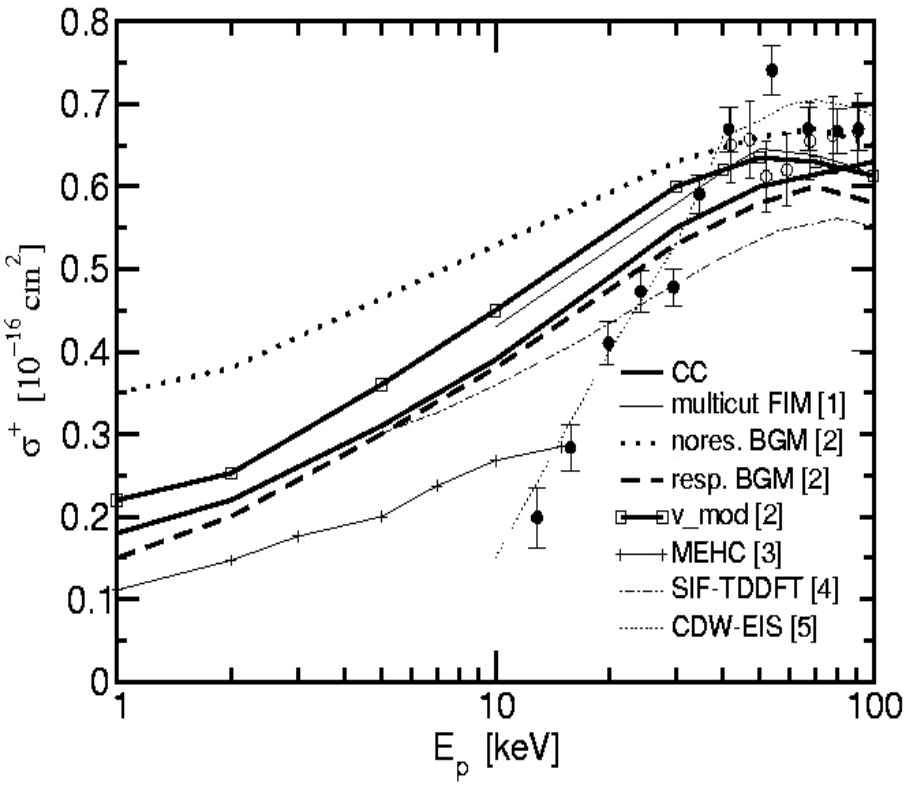
with

$$C_{\lambda j,LM} = \langle \Psi_{\lambda,LM} | \Phi_{j=(\nu,LM)} \rangle .$$

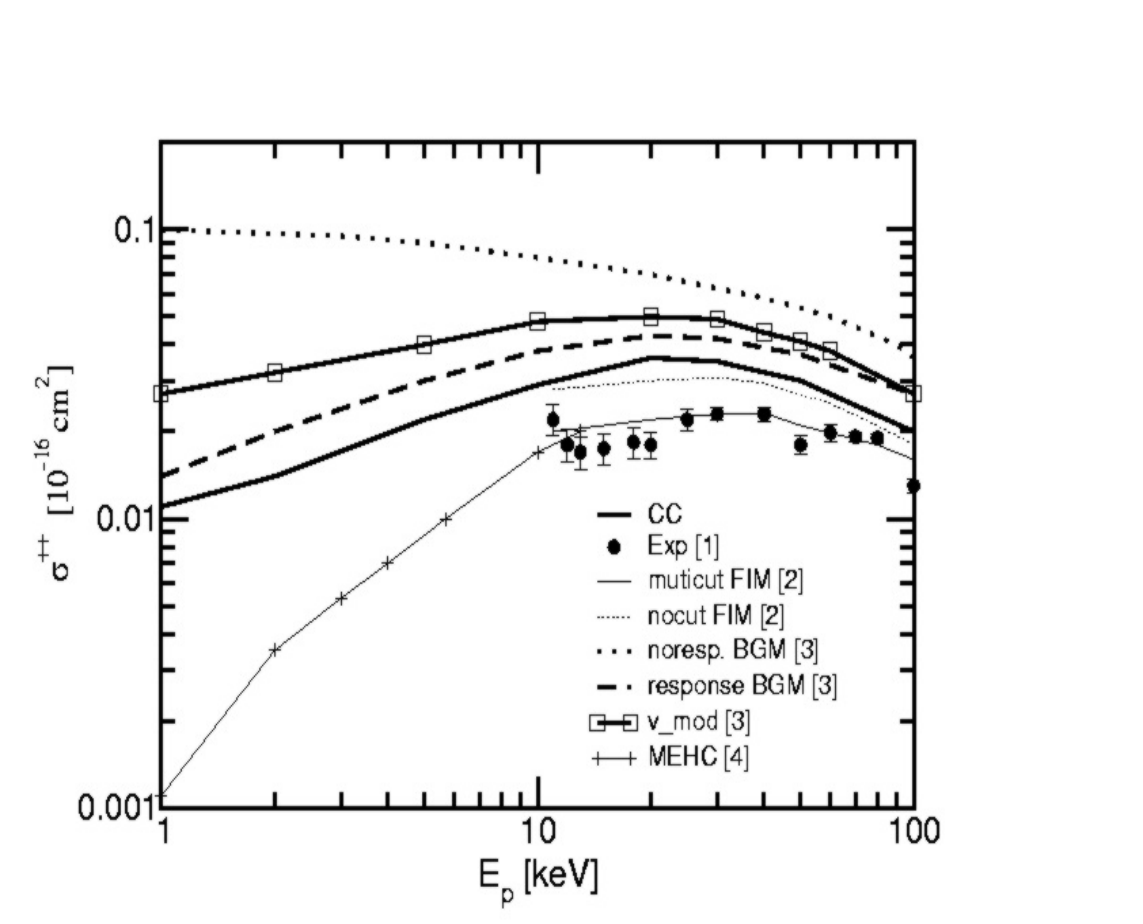
$$A^{\mathrm{bb}}_j = \sum_\lambda |C^{\mathrm{bb}}_{\lambda j,LM}|^2,$$
$$A^{\mathrm{bi}}_j = \sum_\lambda |C^{\mathrm{bi}}_{\lambda j,LM}|^2,$$
$$A^{\mathrm{ii}}_j = \sum_\lambda |C^{\mathrm{ii}}_{\lambda j,LM}|^2,$$

where we assume completeness: $A^{\mathrm{bb}}_j + A^{\mathrm{bi}}_j + A^{\mathrm{ii}}_j = 1.$

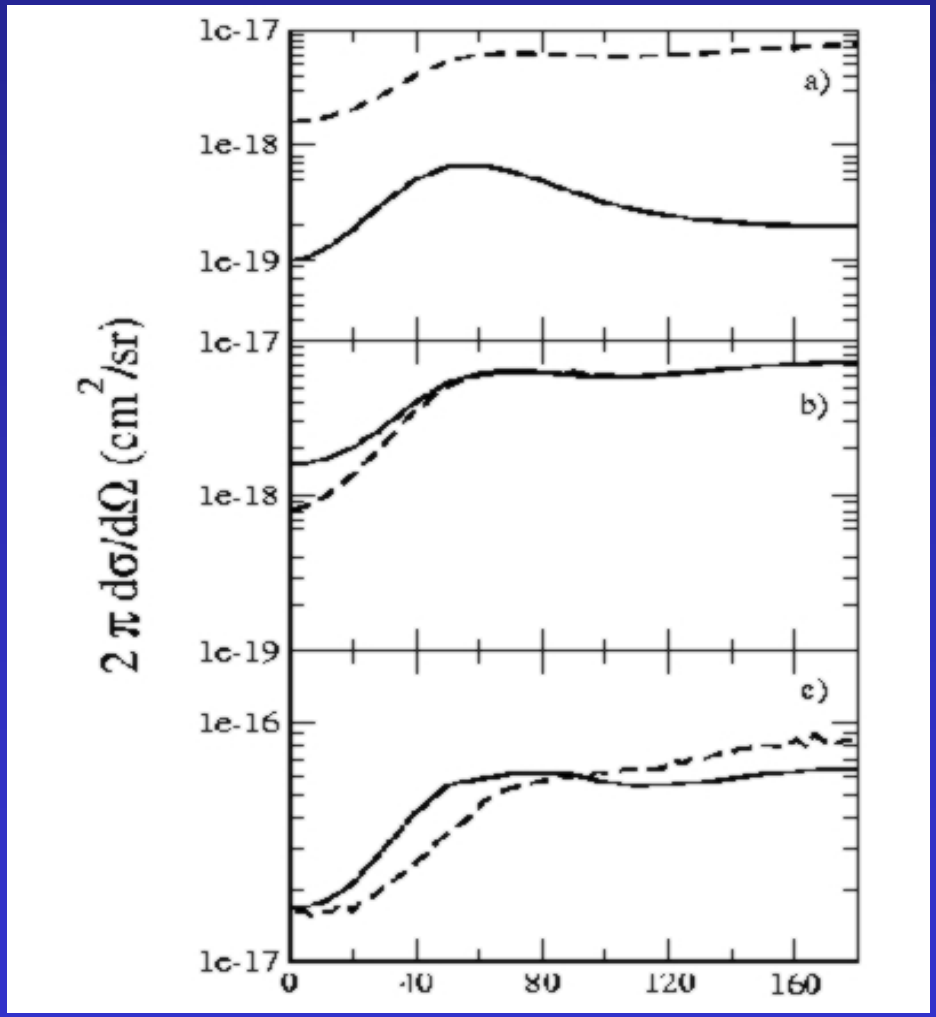
Single ionization total cross sections



Double ionization total cross sections



Angular differential ionization cross section II



10 keV

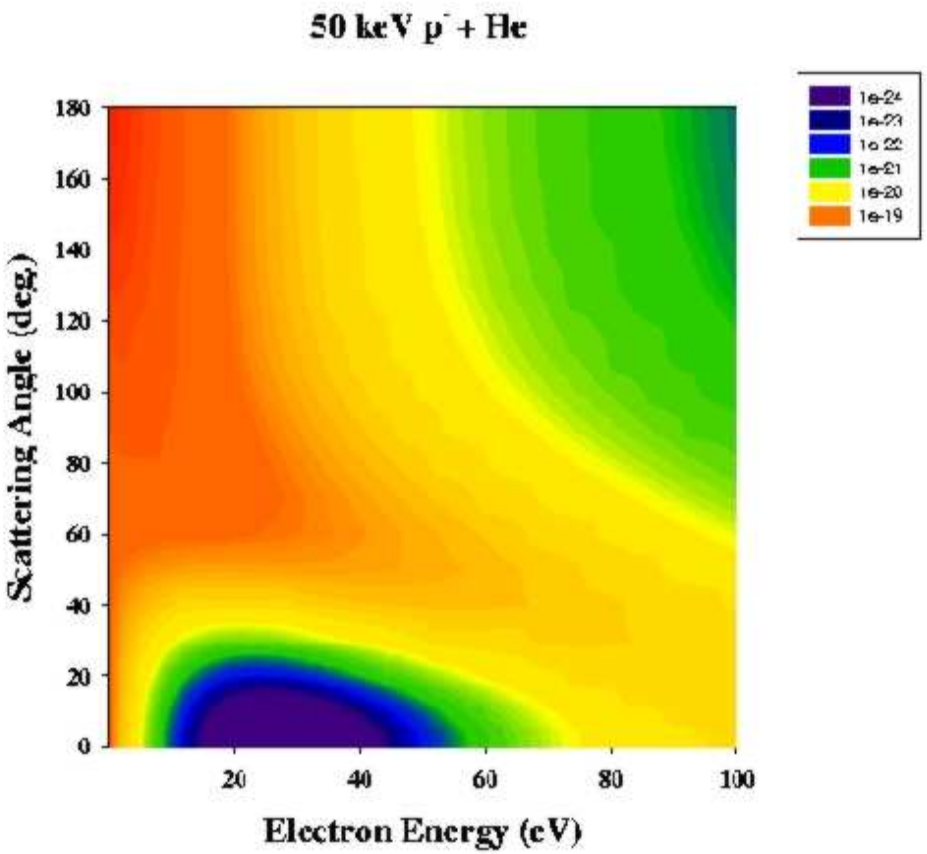
50 keV

100 keV

CC solid line
CTMC dashed line

Electron emission angle

Double differential ionization cross sections



Thank you for your attention!