Ionisation of helium in positron impact

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The Classical Trajectory Monte Carlo method

- Newton's classial non-relativistic equations for 3 and 4 particles

- **3-body CTMC:**
  He^{2+}, e^- and e^+ [1]
  the projectile-electron and the projectile-core interactions are model potential of the form [2]:

$$V(r) = -[(Z-1)\Omega(r) + 1]/r$$

  with $\Omega(r) = [Hd(e^{r/d} - 1) + 1]^{-1}$ Z is the effective charge, d and H parameters from [3]

- **4-body CTMC:**
  four particles are characterised by mass and charges
  all interactions Coulombic
  the interaction between the two active electrons are neglected

- microcanonical ensemble were taken for initial conditions

The Coulomb distorted wave Born approximation model

- our model [4] is defined by the Hamiltonian:

$$H = -\frac{1}{2}\nabla_p^2 + H_{He} + V_{p-He}$$

- the unperturbed helium Hamiltonian:

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

- the projectile-electron interaction:

$$V_{p-He} = \frac{2}{R} - \frac{1}{|\mathbf{R} - \mathbf{r_1}|} - \frac{1}{|\mathbf{R} - \mathbf{r_2}|}$$

- coupled channel expansion:

$$\Psi(\mathbf{r_1}, \mathbf{r_2}, \mathbf{R}) = \sum_{\mathbf{n}} \varphi(\mathbf{R_n})\Phi_{\mathbf{n}}(\mathbf{r_1}, \mathbf{r_2},)$$

- the angular-differential cross section:

$$\frac{d\sigma}{d\Omega} = |f_n(\theta, \vartheta)|^2 = \frac{4\pi^2\mu^2 k_0}{k_n} \int\int\int d\mathbf{r_1} d\mathbf{r_2} d\mathbf{R}$$

$$\sum_n \varphi_n^*(\mathbf{R})\Psi_n^*(\mathbf{r}_1, \mathbf{r}_2)[\, V_{p-He} - 2/R\,]$$

$$\times\varphi_0(\mathbf{R})\Psi_g(\mathbf{r}_1, \mathbf{r}_2)$$

The wave function of the helium atom

Configuration Interaction expansion of $\Phi_j(\mathbf{r_1}, \mathbf{r_2})$ in terms of two-particle basis functions f_μ

$$\Phi_j(\mathbf{r_1}, \mathbf{r_2}) = \sum_\mu \mathbf{b}^{\mathbf{j}}_\mu \mathbf{f}_\mu(\mathbf{r_1}, \mathbf{r_2}).$$

where $f_\mu(\mathbf{r_1}, \mathbf{r_2})$ are symmetric (S=0) products of

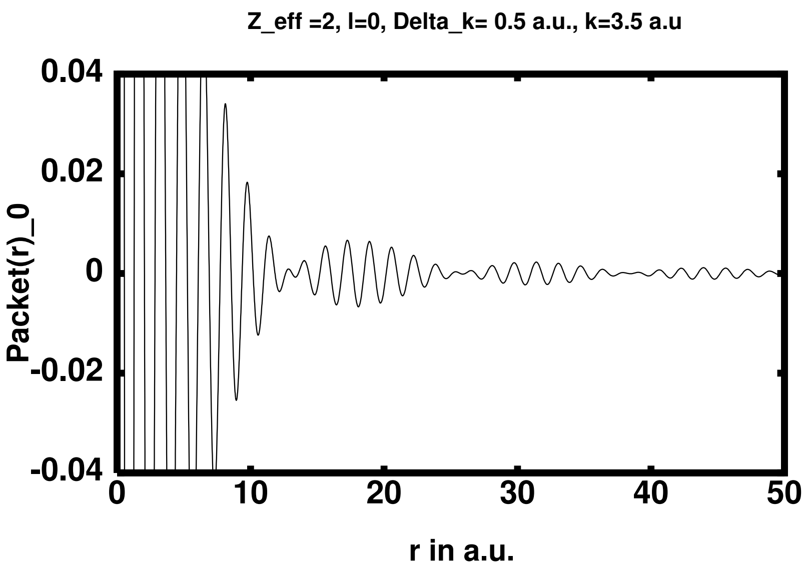
- Slater-type orbitals:

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

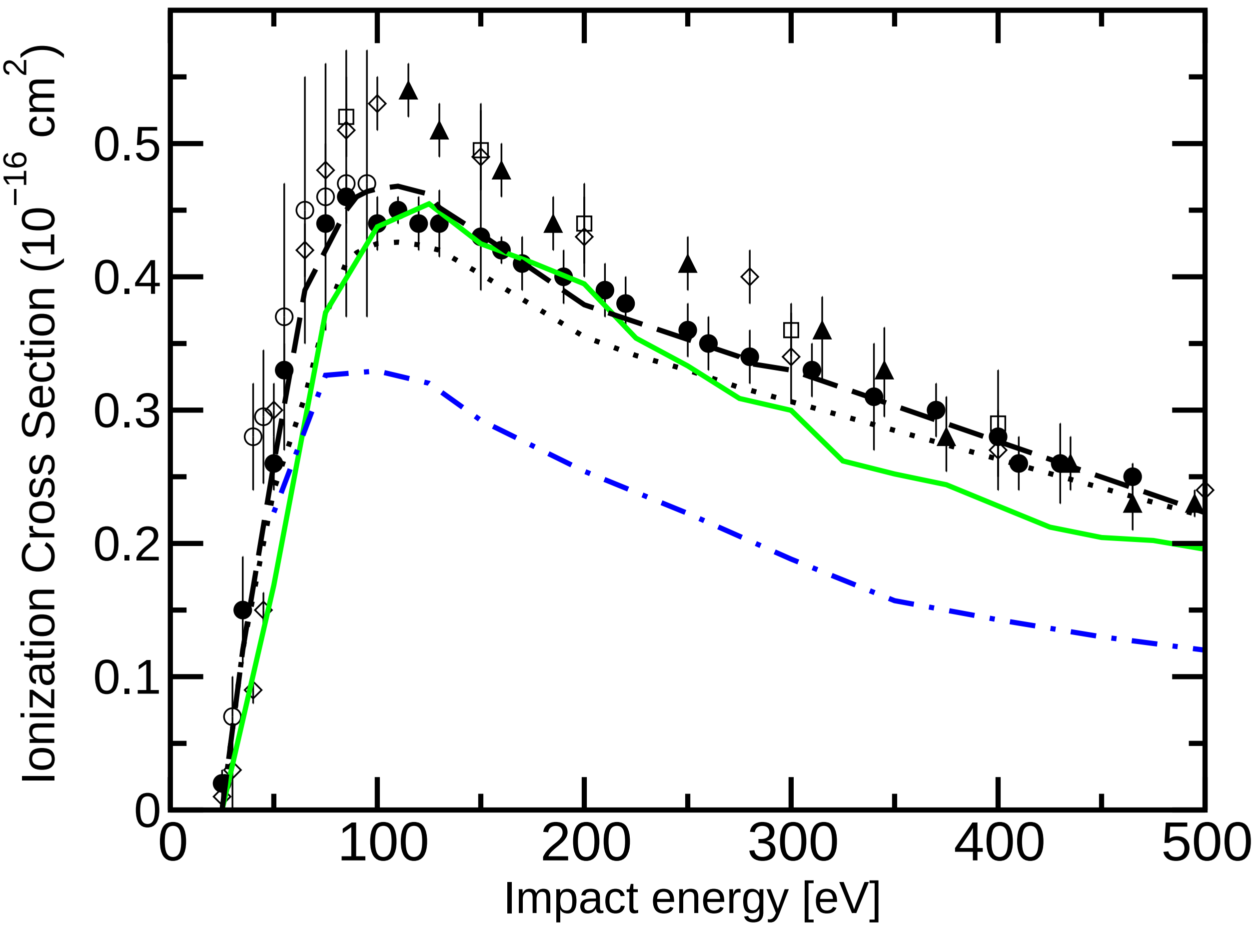
- regular Coulomb wave packets:

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

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



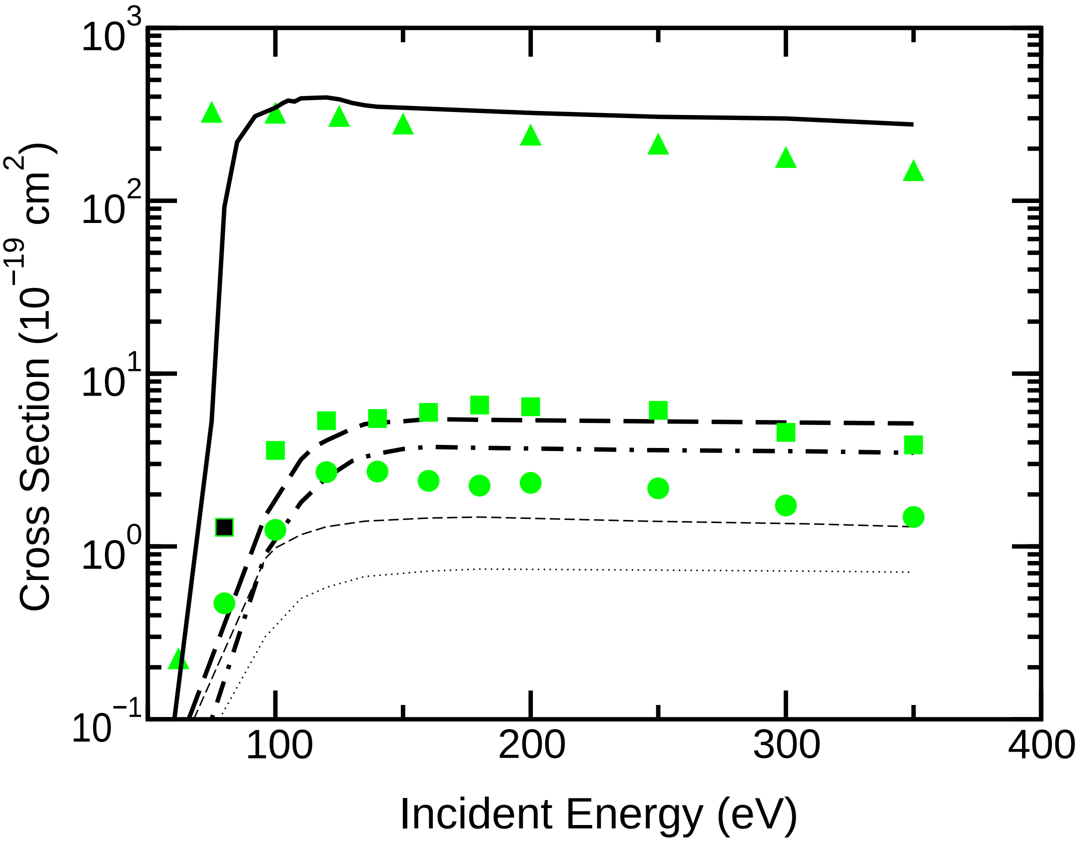
Results for total ionisation



Positron impact ionization cross sections of helium.
Experimental data: (◇) Knudsen et al. [5]; (▲) Moxom et al. [6]; (●) Fromme et al. [7]; (○) Mori and Sueoka [8]; (□) Jacobsen et al. [9].
The solid line presents **3B-CTMC** and the dash-dotted line stands for **4B-CTMC** results. The dashed curve shows our distorted wave results and the dotted line presents the work of Campeanu *et al* [10].

Results for partial ionisation

$$e^+ + He(1s1s) \rightarrow He^+(1s) + e^+ + e^- \quad (A)$$
$$e^+ + He(1s1s) \rightarrow He^+(2s) + e^+ + e^- \quad (B)$$
$$e^+ + He(1s1s) \rightarrow He^+(2p) + e^+ + e^- \quad (C)$$



Ionisation cross sections of helium where the helium ion is in a well defined state Eq. (A-C). The three full symbols stand for our **3B-CTMC** results, ▲ for (A), ■ for (C) and (•) for (B). The thick lines represent our distorted wave results. The solid line is for (A), dashed line for (C) and the dash-dot-dashed line is for (B).
The dotted thin line shows the results of Moores [11] for (B) and the thin dashed line stands for (C).

Summary

- we presented a comparative study for ionisation of helium in positron impact
- our **3B-CTMC** and Coulomb distorted wave Born model are in good agreement with experimental data
- our **4B-CTMC** model gives 60 percent smaller results than the experimental data, this is due to screening effects
- partial ionisation cross sections are also presented and compared with different theoretical results
- we hope that our work stimulates experimentals to measure the processes mentioned above

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