# State-selective charge exchange cross section in $Be^{4+}$ +H(1s) collision


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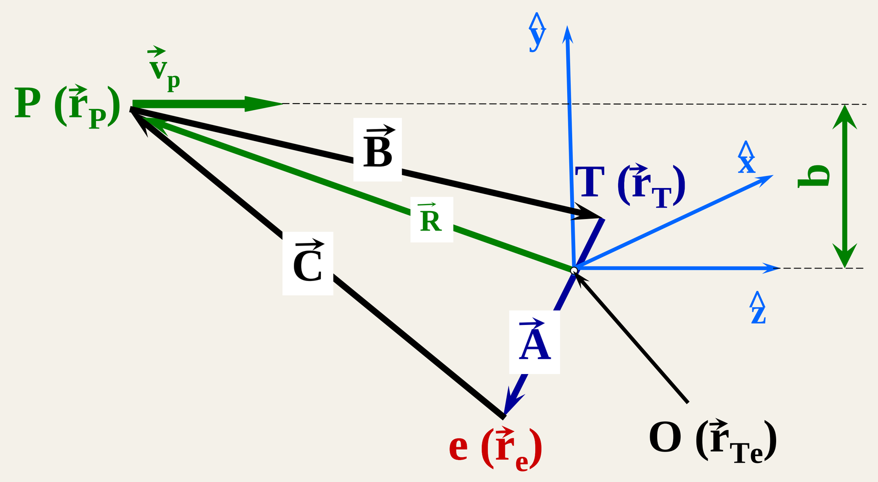
## Abstract

State-selective charge exchange to the projectile bound state cross sections is calculated for collision of $Be^{4+}$ with ground state hydrogen using the 3-body classical trajectory Monte Carlo method (CTMC) and quasiclassical trajectory Monte Carlo method of Kirschbaum and Wilets (QTMC-KW). The cross sections are obtained for projectile *nl* = 3s, 3p, 3d states. Calculations are carried out in the impact energy range between 1 and 1000 keV/amu. Our results are compared with previous theoretical results. We show that the calculations by QTMC-KW model significantly improve the calculated cross sections.


## Introduction

Beryllium is typically considered as the armor material for Plasma Facing Components (PFCs) of fusion devices and it is the first wall of the International Thermonuclear Experimental Reactor (ITER) (Pitts et al. 2011). The inelastic collision processes between $Be^{q+}$ ions and H are particularly important when energetic neutral hydrogen is injected into the plasma for heating and diagnostic purposes (Hackman et al. 1984). Therefore the accurate description and knowledge of these interactions are extremely important for fusion research. The state-selective cross sections for charge exchange in collision between Be and hydrogen atom has been studied in the past using different theoretical approaches such as; MOCC method (Harel et al. 1998, 1997), AOCC method (Fritsch et al. 1984), OEDM (Errea et al. 1982, 1998) and GTDSE method (Jorge et al. 2016). The quasiclassical trajectory Monte Carlo method of Kirschbaum and Wilets) (Kirschbaun et al. 1980) is one step further for a better description of the classical atomic collisions. For atoms, a necessary condition for stability is that the electrons are not allowed to collapse to the symmetry point, i.e., to the nucleus. The effective potential enforcing this condition motivated by the Heisenberg uncertainty principle $rp > \xi_H \hbar$, where r and p are the distance and momentum of an electron with respect to a nucleus and $\xi_H$ is constant. For the H atom, this condition is equivalent to the de Broglie description of the hydrogen atom. In this work we present state selective charge exchange cross sections in collision between $Be^{4+}$ and ground state hydrogen atom using the 3-body classical trajectory Monte Carlo method and quasiclassical trajectory Monte Carlo method of Kirschbaum and Wilets. Our results are compared with previous theoretical results.

## Theory




$$H_0 = T + V_{coul} = \frac{|\vec{P}_p|^2}{2m_p} + \frac{|\vec{P}_e|^2}{2m_e} + \frac{|\vec{P}_T|^2}{2m_T} + \frac{Z_pZ_e}{|\vec{r}_p - \vec{r}_e|} + \frac{Z_eZ_T}{|\vec{r}_e - \vec{r}_T|} + \frac{Z_pZ_T}{|\vec{r}_p - \vec{r}_T|}$$

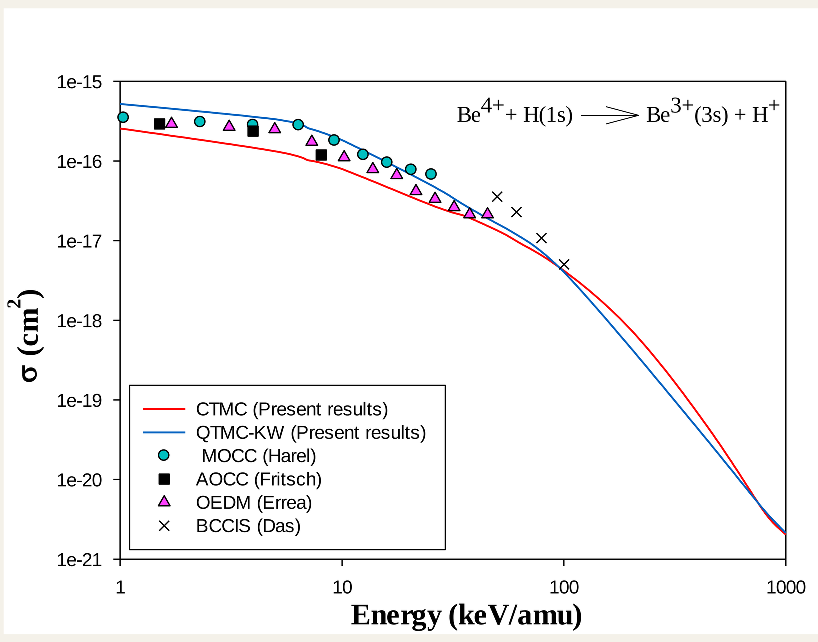
$$H_{FMD} = H_0 + V_H$$

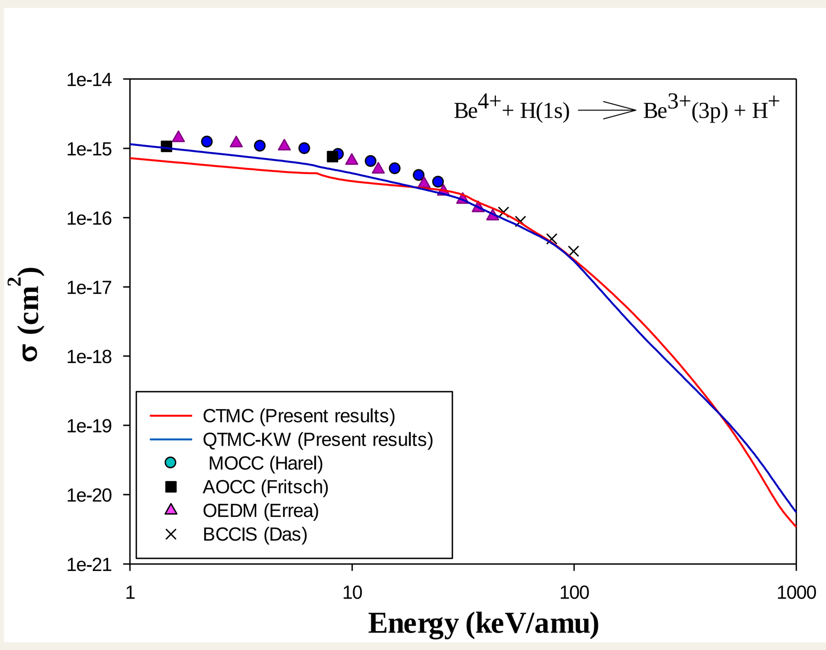
$$V_H = \sum_{n=a,b} \sum_{i=1}^{N} f(r_{ni}, p_{ni}; \xi_H, \alpha_H) \quad \begin{cases} r_{\alpha\beta} = r_\beta - r_\alpha \\ p_{\alpha\beta} = \dfrac{m_\alpha p_\beta - m_\beta m_\alpha}{m_\alpha + m_\beta} \end{cases}$$

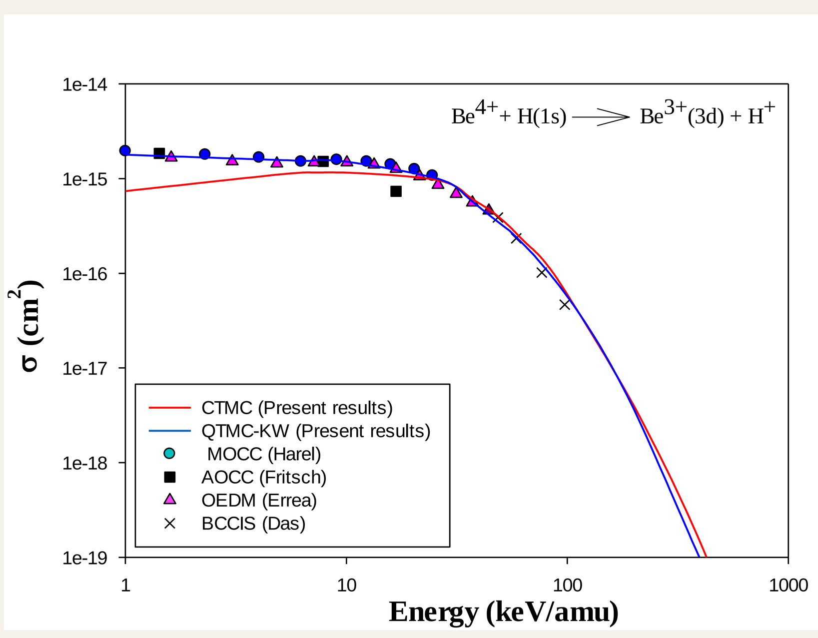
The Heisenberg potential can be written in the following form

$$f(r_{\lambda\nu}, p_{\lambda\nu}; \xi, \alpha) = \frac{\xi}{4\alpha r_{\lambda\nu}^2 \mu_{\lambda\nu}} exp\left\{\alpha\left[1 - \left(\frac{r_{\lambda\nu}p_{\lambda\nu}}{\xi}\right)^4\right]\right\}$$

## Results and Discussion




## Conclusion

We have calculated the state-selective charge exchange cross section to the projectile bound state according to CTMC and QTMC-KW methods. Figures show the state-selective charge exchange cross section into the 3s, 3p, 3d states of the projectile in $Be^{4+}$ + H(1s) collision, respectively. According to Figures, we found improvement in the cross section using QTMC-KW method compared to the standard CTMC model. We also found excellent agreement between our QTMC-KW results and the previous data.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