Monte Carlo Simulation Calculations of Ionization Cross Sections

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In this paper we will describe a program written by Igor Kaganovich to calculate ionization cross sections for collisions between projectile protons on stationary hydrogen nuclei. The program can be easily modified to handle any fully stripped projectile by just adjusting the potential for the heavier ions. The general idea is to simulate the collision using classical trajectory calculations and to sample many different simulations, seeing how often the electron ionizes and then to obtain a probability. We will then present the results of the simulations and compare them with experimental values.

We begin by discussing a few important points within the code without referring to the code itself.

We determine whether the electron ionizes by looking at its energy values and position with respect to the two nuclei after the collision:

$$\text{If } V_p(r_p) > \frac{v_p^2}{2} \text{ and } r_p < r_t \text{ then a charge exchange has occured.}$$

$$\text{If } V_t(r_t) > \frac{v_t^2}{2} \text{ and } r_t < r_p \text{ then the electron remains in the target nucleus.}$$

Here all values with a p are with respect to the projectile and those with a t are with respect to the target nucleus. If neither of these conditions is met we assume that the electron has ionized. The simplicity of this ionization determination method is on the one hand convenient, but on the other hand it does require that we run the simulation long enough so as to assure that the result we determine is correct. This ends up slowing down the program for highly charged projectiles or targets.

The simulation consists of a running Newton's equations with the Runge Kutta method given different sets of initial conditions. Because of conservation of energy and momentum we only need to give four initial coordinates describing the electron - the radius from the stationary nucleus, the two angles in spherical coordinates, and a third angle between the rotational velocity vector and the radius vector. We also set the impact parameter for the collision.

Determining the initial velocity of the electron is slightly tricky. The initial radial velocity, v_r, is calculated using conservation of energy:

$$\frac{v_r^2}{2} + \frac{1}{2}(\frac{l}{r})^2 = -U(r) - I_{n,l}$$

We use conservation of angular momentum, $l = v_\beta r$, to find the rotational velocity v_β:

The rough part is dividing up the radial and rotational velocities into each one's Cartesian components. We define α to be the angle between the vector from the electron to the nucleus and the direction of the rotational velocity. Thus in spherical coordinates the total initial velocity vector is:

$$\begin{pmatrix} v_\beta \cos(\alpha)\hat{\theta} \\ v_\beta \sin(\alpha)\hat{\phi} \\ v_r \hat{r} \end{pmatrix}$$

Now we use rotation matrices to rotate through both ϕ and θ in order to switch from spherical to Cartesian coordinates:

$$\begin{pmatrix} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos(\theta) & 0 & \sin(\theta) \\ 0 & 1 & 0 \\ -\sin(\theta) & 0 & \cos(\theta) \end{pmatrix} \begin{pmatrix} v_\beta \cos(\alpha) \\ v_\beta \sin(\alpha) \\ v_r \end{pmatrix}$$

$$= \begin{pmatrix} v_r \cos(\phi)\sin(\theta) + v_\beta(\cos(\theta)\cos(\phi)\cos(\alpha) - \sin(\phi)\sin(\alpha)) \\ v_r \sin(\phi)\sin(\theta) + v_\beta(\sin(\phi)\cos(\theta)\cos(\alpha) + \cos(\phi)\sin(\alpha)) \\ v_r \cos(\theta) - v_\beta \sin(\theta)\cos(\alpha) \end{pmatrix}$$

and this will be the initial total velocity vector.

Anyhow, there are two methods in which we can assign values to the initial conditions. We can use a stochastic method where the conditions are chosen randomly or we can pick values using a uniform distribution between the minimum and maximum possible values for the conditions and then create a simulation for every permutation of these parameters. If we do the latter method than we'll have to put weights on the probability calculation because if you pick values of θ and ϕ randomly from 0 to π and 0 to 2π , this doesn't leave you with a uniform distribution of points on the surface of the sphere. Instead you are left with clutters of points by the poles. Thus we will want to weigh every sampling by $\sin(\theta)$ so as to weigh down those angles which would have less probability of being chosen randomly. The $\sin(\theta)$ comes from using the microcanonical ensemble for hydrogen like atoms. This is equivalent to creating a distribution that is uniform in $\cos(\theta)$ and this will distribute points uniformly around the surface of the sphere like we want.

However, we must also divide each sampling by the average value of $\sin(\theta)$ from 0 to π so that the total possible probability still equals one. So in all, when accumulating the probability calculation we weigh each trajectory with:

$$\frac{\sin(\theta)}{\frac{1}{\pi}\int_0^\pi \sin(\theta)\, d\theta} = \frac{\pi}{2}\sin(\theta)$$

We can do this for the stochastic method as well, or alternatively we can create a random number generator that will give us a uniform distribution on the surface of a sphere. We do this by simply picking a random number between -1 and 1 and then plugging it into the inverse cosine function to give a distribution uniform in $\cos(\theta)$.

Since we are ultimately interested in finding the ionization cross section, every time a trajectory results in an ionization we add the following to the running sum:

$$\sigma = \frac{2\pi P(\rho)\rho\rho_{max}}{N} = \frac{\sin(\theta)\pi^2\rho\rho_{max}}{N}$$

where ρ is the impact parameter and N is the number of total trajectories that will be simulated. In the stochastic method, this is simply the amount of times the program runs through the code, and for the unifrom mesh method, N is the amount of permutations of initial conditions that we allow for. It is expected that both methods should be equivalent when enough trajectories are used.

The factor $\frac{\rho_{max}}{N}$ replaces the $d\rho$ in the cross section integral. ρ_{max} is chosen at the approximate value of ρ for which the probability that the particle will ionize becomes zero.

Results

Using a classical trajectory Monte Carlo (CTMC) simulation we calculated ionization and charge exchange cross sections for collisions of various ion projectiles on hydrogen and helium targets. Below are the results for hydrogen, where all the cross sections are normalized.

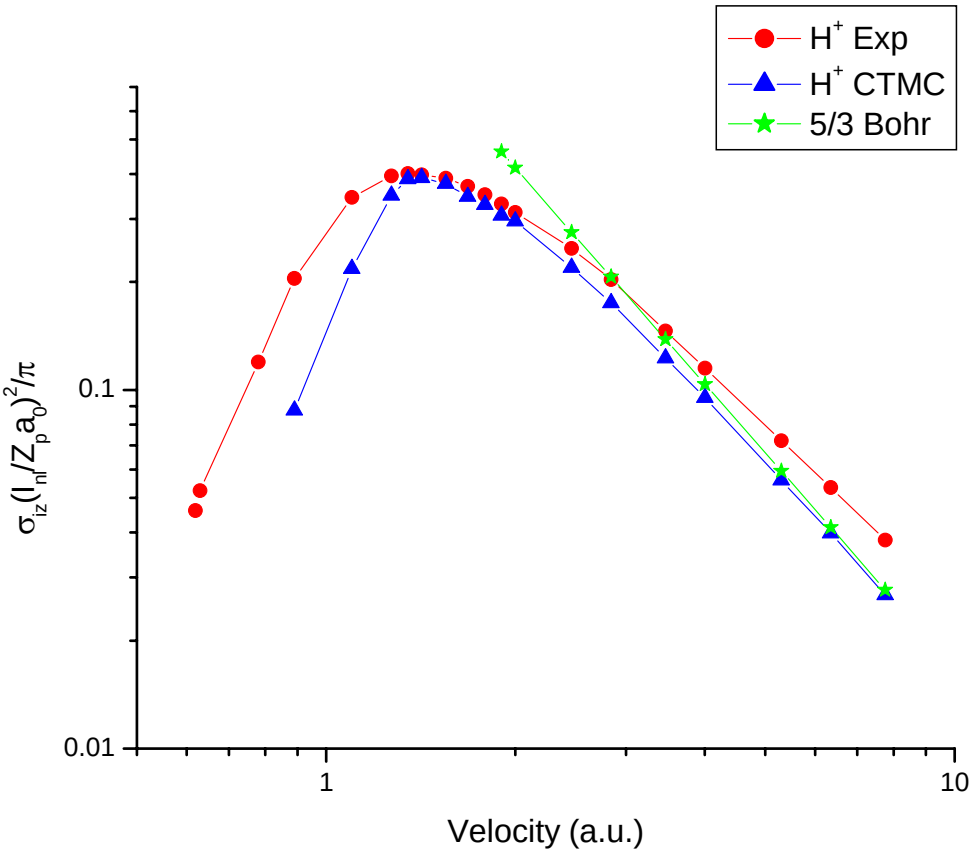

Figure 1 - This is a proton on hydrogen collision. The maximum impact parameter for these runs was 5.5 au. The experimental results come from [1,3].

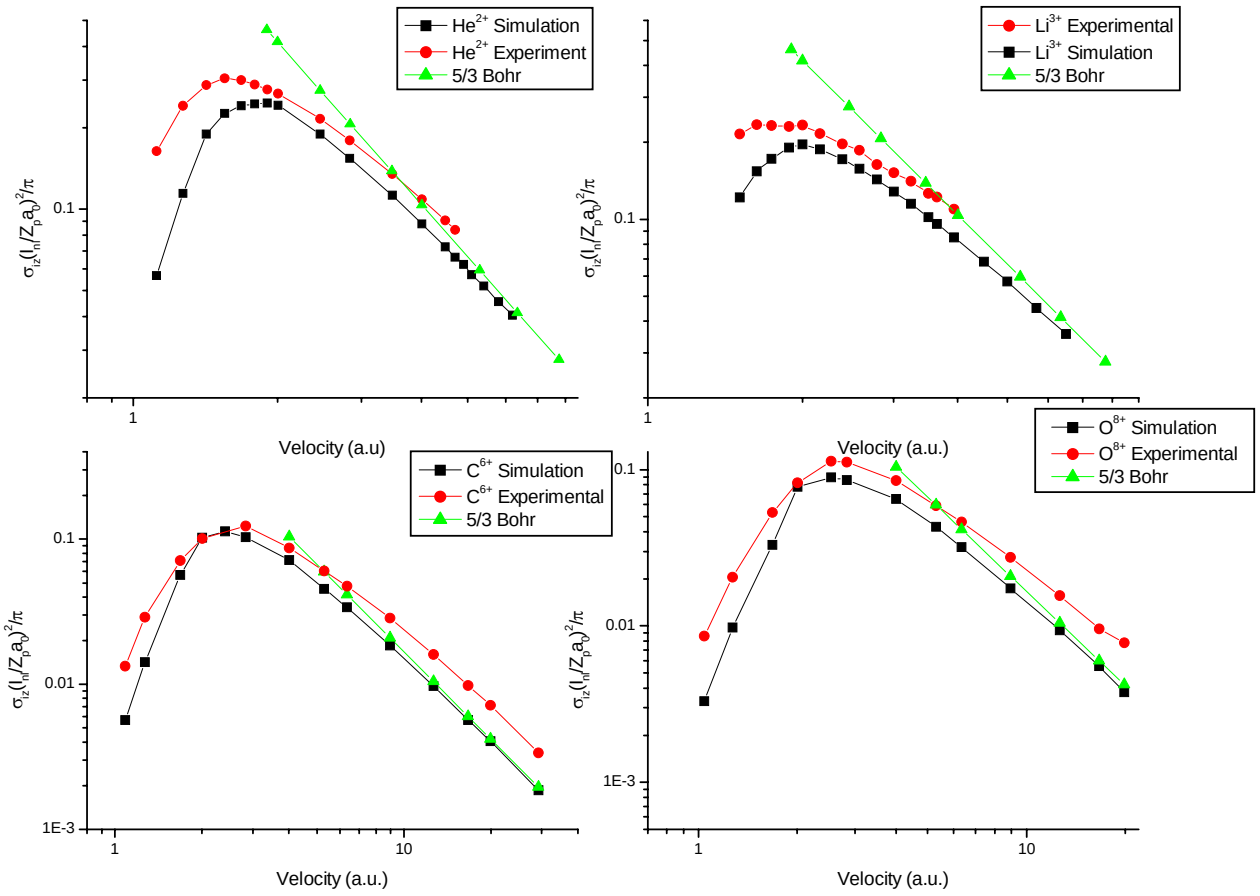

Figure 2 – Normalized ionization cross sections of fully stripped ions on hydrogen. The experimental results for He, Li, and C and O come from [1],[2], and [6] respectively.

For most runs with hydrogen targets we used an initial separation distance of 25 au. For the bigger ions such as oxygen and carbon this distance was increased when doing runs of lower velocities because the larger charge means that the projectile can start drawing in the electron from much farther away.

The simulation results always underestimate the experimental results. This is largely due to the fact that the classical simulation does not account for instances of ionization that result from quantum mechanical phenomena. However, for the most part, both curves peak at around the same maximum velocity. For velocities between 1.3 and 2.3 au our simulation seems to be a good approximation of experimental values, coming within 10% in the proton on hydrogen case. A stochastic method of choosing initial coordinates for the simulation was used for these results and each case was approximated using 100,000 trajectories (except for the proton runs where we used 150,000 trajectories). The maximum value of the impact parameter for He, Li, C, and O was 5.7, 6.5, 11, and 12 au respectively.

A good way to see if the simulation is running correctly is to compare it to the 5/3 Bohr approximation at high velocities [7]:

$$\sigma = \frac{5}{3} B_{nl} \sigma^{Bohr}$$

where $\sigma^{Bohr} = 2\pi \frac{Z_p^2}{v^2 I_{nl}}$ and $B_{nl} = \frac{3}{5}\left(\frac{2K_{nl}}{3I_{nl}} + 1 \right)$.

This approximation is essentially the maximum bound for cross sections using classical methods and it is only valid for high velocities. Indeed, the graphs above show that the CTMC's meet this line at the limit of high velocities.

We also calculated charge exchange cross sections using the CTMC method:

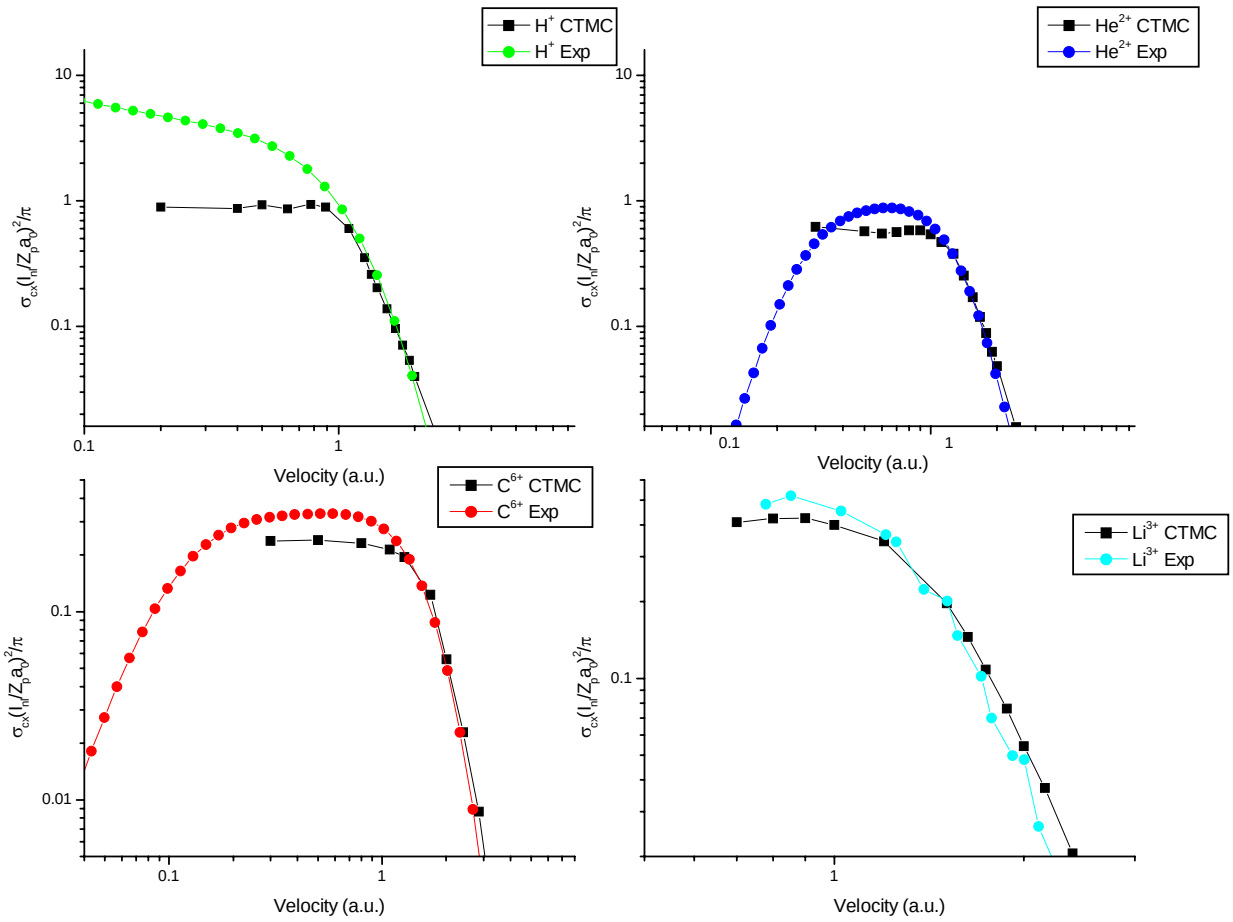

Figure 3 – Charge exchange cross sections of fully stripped ions on hydrogen. The experimental results are from [1] for H and He, [2] for Li, and [6] for C.

We also tried some simulations using heavier projectiles, such as argon and gold ions. With highly charged ions as large as gold, it has been shown [17] that you can neglect the ion's electrons' contributions to potential and treat the projectile as if it were a fully stripped ion of the same charge. With smaller ions like argon, the electrons surrounding the ion can have noticeable effect on the potential from the projectile so we used approximations of the potential such as this one, which was used for Ar+7:

$$V(t) = V_{\alpha}(r) + \frac{Z_{ion}}{R_{ion}}$$

where

$$V_{\alpha}(r) = \frac{Z}{r} K_s \left(\frac{r Z^{\frac{1}{3}}}{b} \right)$$

and

$$K_s(x) = \left[1 - \left(\frac{x}{S_1} \right)^3 \right] . \frac{1}{\left(1 + 0.02747\sqrt{x} + 1.243x - 0.1486x^{1.5} + 0.2302x^2 \right)}$$

and $Z = 18, Z_{ion} = 3, R_{ion} = 1.3383, b = 0.8853,$ and $S_1 = 3.96175.$

Here we show the normalized results of two Ar ions compared with some of our previous results:

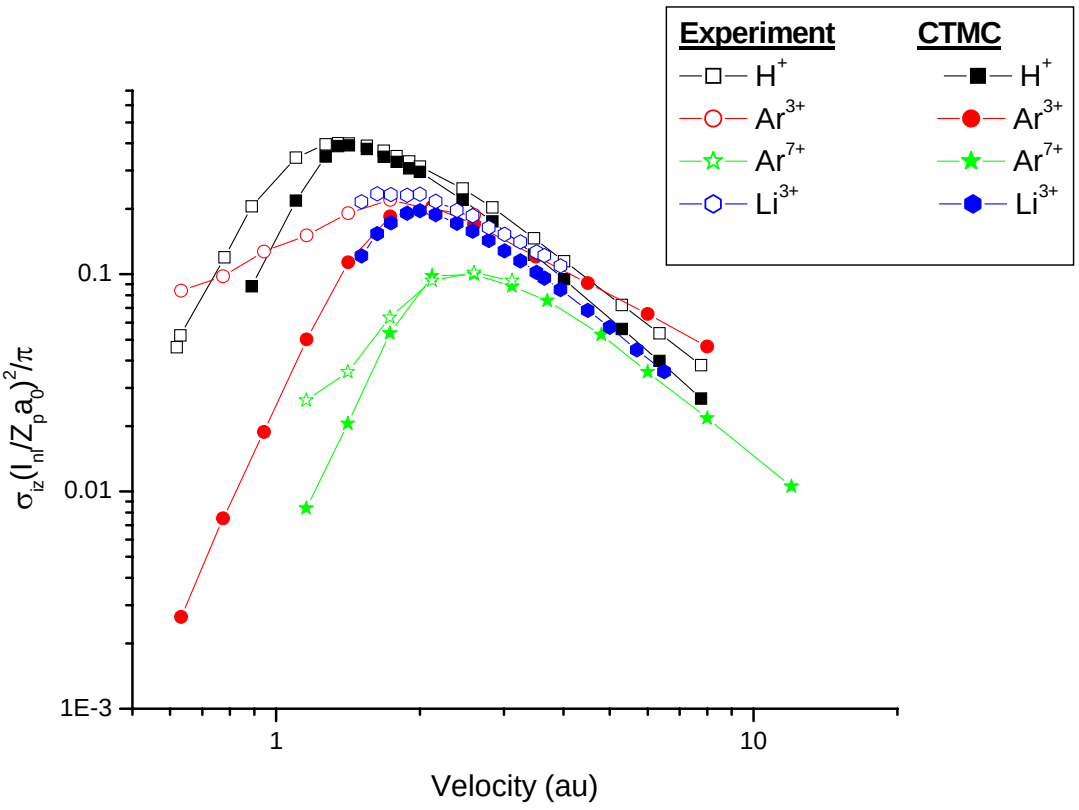

Figure 4 – Ionization cross sections of some fully stripped ions and other heavier ions on atomic hydrogen. The experimental values for the Ar ions were taken from [14].

For the most part the two Ar cross sections resemble the others in their basic shape and curvature. For instance, notice the similarities between Li+3 and Ar+3. One oddity is that the Ar+3 cross section does not approach the 5/3 Bohr limit at high velocities, unlike those of the other ions. Another problem here is that the experimental results do not have the same basic shape as any of the others. This is due to the large amount of ionization that occurs at low energies called auto-ionization that is only accounted for with quantum mechanic methods. For all the simulations we used a maximum impact parameter of 10 au. For most points we ran 100,000 trajectories but for lower velocities of the Ar+3 ions the simulation was extraordinarily slow so we did up to half as many.

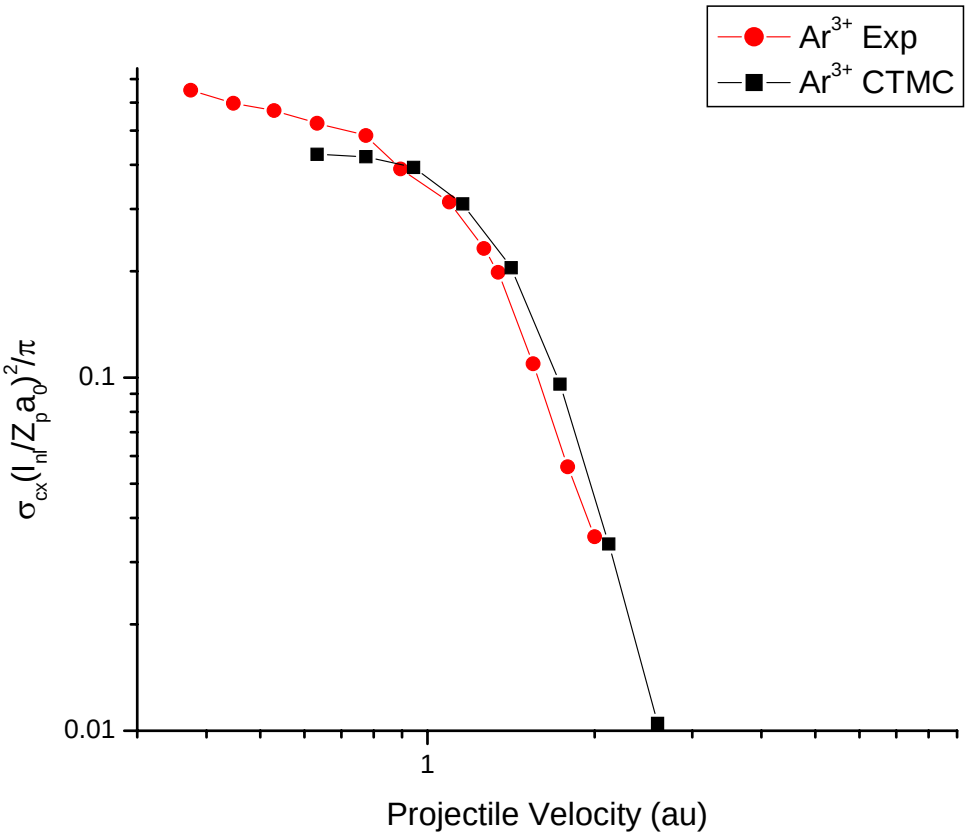

Figure 5 – Normalized charge exchange for Ar+3 ions on hydrogen. Experimental values from [14].

Helium Targets

We altered the hydrogen code slightly to approximate helium target cross sections as well. Since there are two electrons their interactions with one and another must be taken into consideration. We made use of Shevelko's approximation of the total potential of the target (the two protons and one electron),

$$V(r) = (r\beta + 1)\frac{(\zeta e^{-2r\beta})}{2r} + \frac{1}{r}$$

Where $\beta = 1.65$ and $\zeta = 2$.

Also, since there are two electrons that can be ionized, the total cross section is multiplied by a factor of two. The ionization potential for neutral He is 0.904 au.

Below are results for the helium targets:

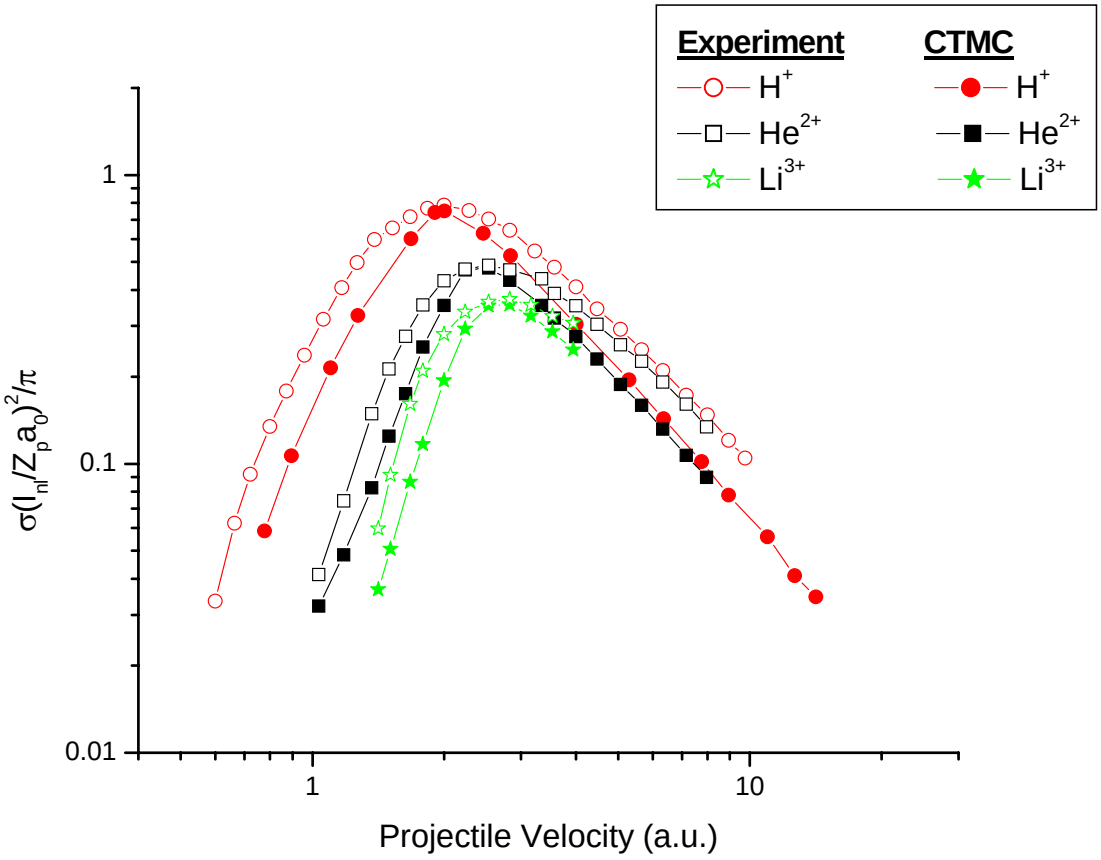

Figure 6 – The normalized ionization cross section for fully stripped ions on Helium targets. Experimental values come from [4,5].

Again, the CTMC results all converge to 5/3 Bohr limit (not shown) at high velocities.

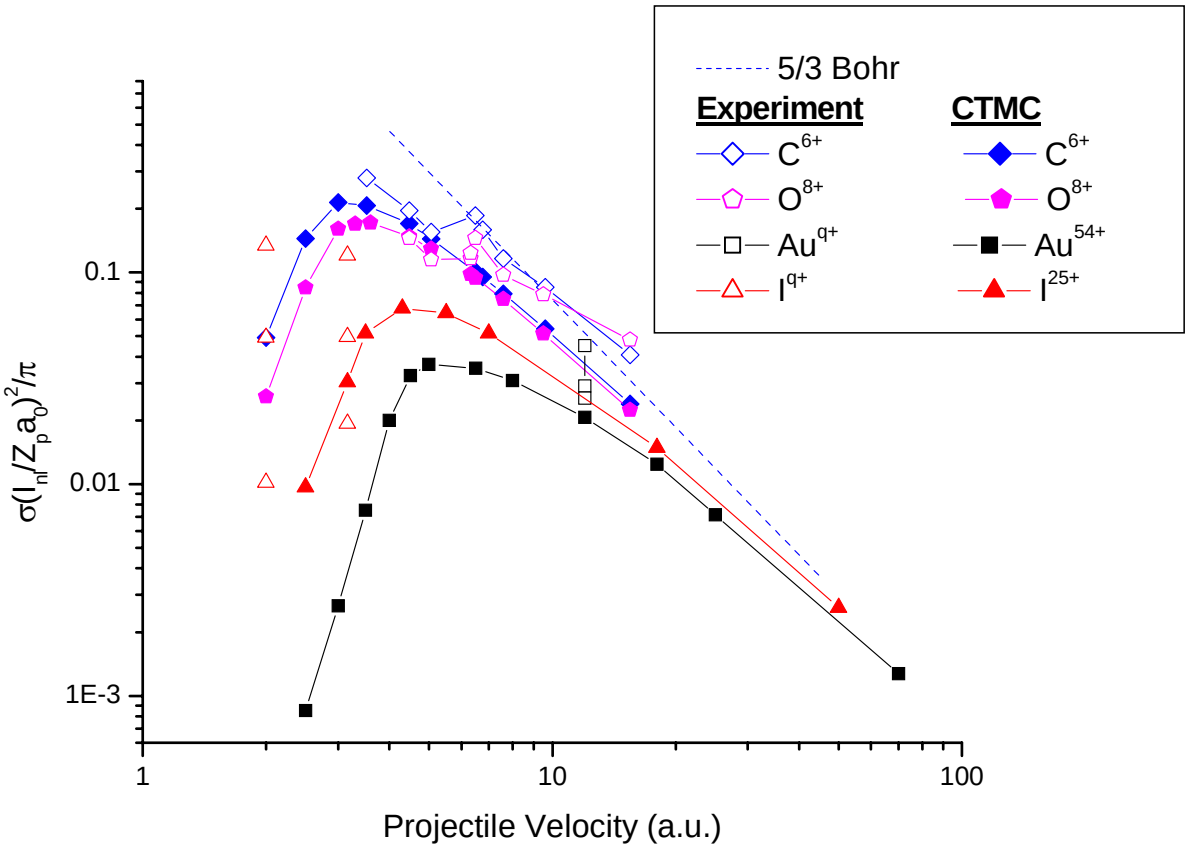

Figure 7 – Ionization cross sections for larger fully stripped ions and even larger non-fully stripped ions on He targets. The experimental data (which doesn't seem to be calibrated properly) is from [8-13] for O and C, and I and Au are from [15] and [16] respectively.

This is a sampling of some the larger charges we worked with. For the gold and iodine simulations, we treat the projectiles as if they were fully stripped ions of the same charge. We are able to ignore the effects of the electrons in these projectiles because almost all ionization occurs at impact parameters for away from the target [17]. It was hard to find experimental data and the data we did find do not seem to be too reliable as you may be able to tell by looking at Fig. 7. The experimental data includes many different charged ions as opposed to our data which shows just one charged ion over many different velocities. The three gold ions shown have charges of 24, 43, and 54, whereas the Iodine ions have charges of 5, 10 (the highest), and 16 (the lowest) at a velocity of 2 in au and 9, 15, and 25 (from lowest to highest) at a velocity of 3.16. The maximum impact parameter for C, O, Au, and I was 6, 8, 30, and 20 au respectively. For the Au simulations we used an initial separation distance of 65 au instead of the usual 25 au because the large charge seemed to be affecting the electron from much farther away.

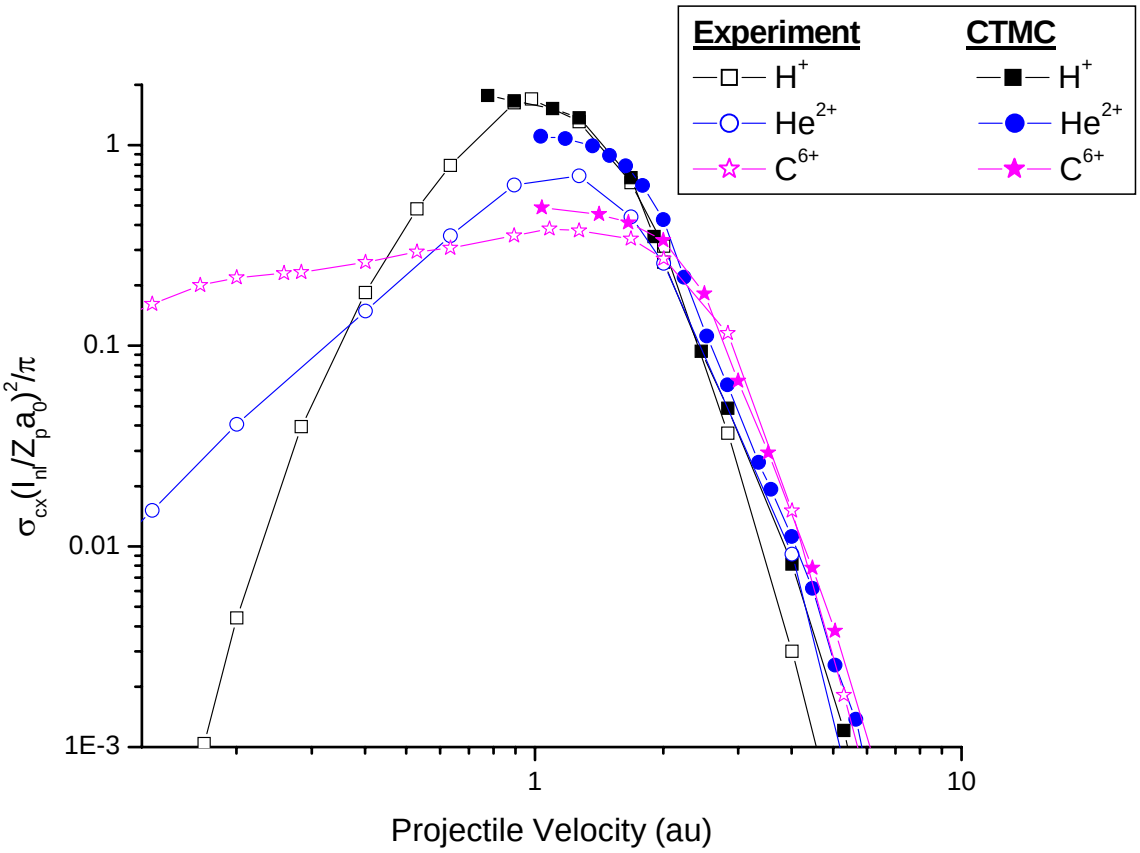

Figure 8 – Charge exchange cross sections of ions on He targets. Experimental data for H and He are from [1] and for C is from [6].

As you can see from the graph, the simulation matches experimental results nicely in velocities between and 1 and 3 au.

References

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