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LETTER TO THE EDITOR

Electron capture and ionisation in H^+, He^{2+} + Li collisions

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Abstract. Single electron capture and ionisation cross sections have been calculated for H^+ + Li and He^{2+} + Li collisions at energies ranging from 50 to 400 keV amu^{-1}. Double electron capture cross sections are presented for the He^{2+} + Li system. The classical-trajectory Monte Carlo method and the independent-electron model were used to calculate the cross sections. In the energy range investigated, the ionisation process is dominated by electron removal of the valence Li(2s) electron, whereas the single and double electron capture processes are the result of capture from the K shell of the lithium atom.

The scattering of H^+ and He^{2+} ions off a lithium atom target poses the interesting problem of determining the importance of electron capture and ionisation from both the tightly bound K shell and the loosely bound valence-electron shell of the atom. At intermediate energies, both electron shells participate in the collisional processes. This makes it necessary to develop and test a theoretical model that incorporates the electron shell structure. In addition, the double electron capture cross sections for He^{2+} + Li are required to assess the feasibility of a proposal (Post *et al* 1979) that a neutral lithium atom beam be used to probe the alpha particle distributions in Tokamak fusion reactors. After double electron capture, the resulting helium atoms can escape from the plasma fields and be analysed by conventional means.

In this paper, we present the cross sections calculated for single electron capture and for the ionisation collisions of lithium atoms by H^+ and He^{2+} ions,

$$\begin{Bmatrix} H^+ \\ He^{2+} \end{Bmatrix} + Li \begin{cases} \rightarrow \begin{Bmatrix} H^\circ \\ He^+ \end{Bmatrix} + (Li^+) & (1) \\ \rightarrow \begin{Bmatrix} H^+ \\ He^{2+} \end{Bmatrix} + (Li^+ + e) & (2) \end{cases}$$

and for the double electron capture reaction,

$$He^{2+} + Li \rightarrow He + (Li^{2+}). \tag{3}$$

We are interested in the collision energy range from 50 to 400 keV amu^{-1}. In our calculations, we did not account for the electron cascade effects that follow the collisions, consequently we are uncertain about the lithium product states. This uncertainty is denoted by the parentheses in reactions (1) to (3).

In calculating the cross sections, we used the three-body, classical-trajectory, Monte Carlo (CTMC) method (Abrines and Percival 1966, Olson and Salop 1977) to determine the single-electron transition probabilities for electron capture and ionisation and used a hydrogenic model to simulate the two electron shells of the lithium atom target. We employed the Hartree–Fock calculations of Fischer (1977) for the binding energies,

BE, and the expectation values, $\langle R \rangle$, for the $1s^2$ and the 2s electrons of the lithium atom. From these values, we were able to ascribe an effective charge, Z_{eff}, for the lithium atom nucleus that encompasses the screening effects of the electrons. For the K shell, $\langle R \rangle = 0.57\ a_0$ and BE = 2.48 au, we found that $Z_{\text{eff}} = 2.83$, while for the 2s electron $\langle R \rangle = 3.87\ a_0$ and BE = 0.196 au, so that $Z_{\text{eff}} = 1.52$. We performed the CTMC calculations for each collision energy, once with the K-shell parameters and once with the valence-electron parameters.

We then utilised the two sets of calculated single-electron transition probabilities in the independent-electron model (IEM) of Hansteen and Mosebekk (1972) and McGuire and Weaver (1977) to obtain the probabilities for one- two- and three-electron transitions. By defining either the electron capture or the ionisation transition probabilities from the CTMC method as p_K for the K shell and p_L for the 2s electron, we obtained from the IEM framework the probability for a one-electron transition,

$$P_1 = (1-p_L)[2p_K(1-p_K)] + p_L(1-p_K)^2 \tag{4}$$

a two-electron transition,

$$P_2 = (1-p_L)p_K^2 + p_L(2p_K(1-p_K)] \tag{5}$$

and a three-electron transition,

$$P_3 = p_L p_K^2.$$

We integrated the probabilities over the impact parameter to obtain the representative cross sections.

One requirement for the validity of the IEM is that the target atom can be well described as a product of single particle wavefunctions as in the Hartreee–Fock method. For this problem, however, a more important requirement is that the collision be 'sudden' so that the electrons do not have sufficient time during the collision to orbit the nucleus and increase their binding energy as electrons in the same shell are removed. This consideration is especially pertinent for one of the processes under study: the He^{2+} double electron capture reaction.

The radius of the collision region for double electron capture from the K shell of a lithium atom is about $2.5\ a_0$. Therefore, the collision time is comparable with the time required for a K-shell electron to orbit the nucleus at energies around 100 keV amu^{-1}. To assess this effect on the cross section for reaction (3), we performed a third set of calculations with the K-shell parameters equal to the hydrogen-like $He^+(1s)$ ion in which $Z = 3.0$ and BE = 4.5 au. In the energy range investigated, we found that the electron capture of the Li(2s) electron makes a small contribution to double capture. Consequently, we were able to set $p_L = 0$ for the two-electron transition probability given by equation (5) and obtain $P_2 = p_K^2$. We were then able to estimate the effect of sequential capture from the K shell by evaluating the double electron transition probability, $P_2 = p_{K_1} p_{K_2}$, in which single electron probabilities are used with one K-shell electron bound by −2.48 au and the other by −4.5 au.

In calculating the double electron capture, we could use only the single electron transition probabilities for K-shell capture into He^{2+}, because double capture into an excited level leads to autoionisation and produces singly charged He^+ and an ejected electron. As a result, we binned the CTMC single electron capture probabilities (Olson 1981) to account for this effect.

The results for the $H^+ + Li$ system are presented in figure 1. The ionisation cross section is dominated by the removal of the valence, Li(2s), electron. The contribution

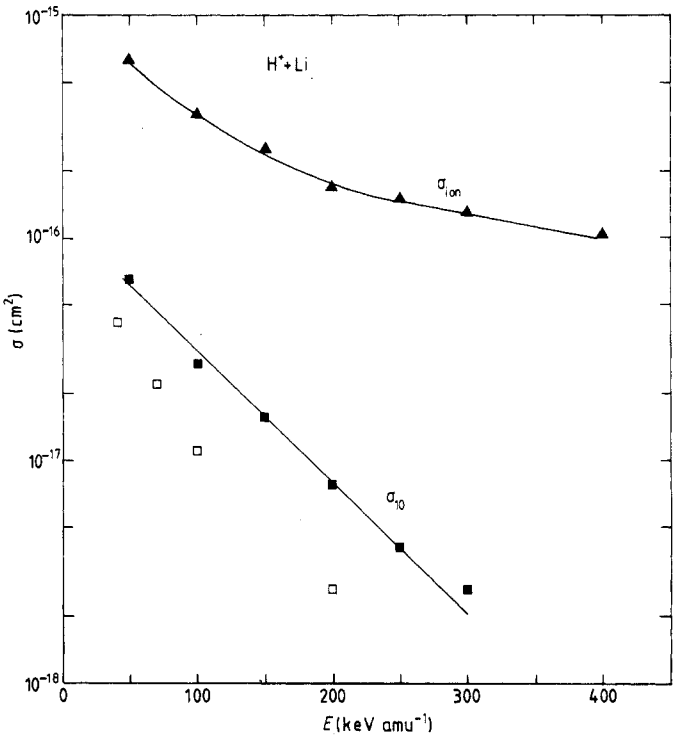

Figure 1. Calculated single electron capture and ionisation cross sections for the $H^+ + Li$ system: full squares and triangles, respectively. Experimental electron capture data from the review by Barnett *et al* (1977) are denoted by open squares.

made by removing a K-shell electron is negligible at low energies (<1% at 50 keV) but rises with increasing energy to approximately 15% of the total at 400 keV. There are no experimental data for testing theoretical ionisation values. We found that the single electron capture cross section for $H^+ + Li$ is almost entirely (>99%) due to the capture of a K-shell electron rather than a lithium valence-shell electron at the highest energies. At lower energies, the contribution from K-shell capture is about 90% at 100 keV and decreases to around 62% at the lowest energy of 50 keV. At 25 keV (not shown), the roles reverse, and capture from the valence shell dominates and contributes approximately 86% to the cross section. Our calculated values are approximately a factor of two to three times larger than the experimental values given in a review by Barnett *et al* (1977). The accuracy of the experimental cross sections is listed as 'unknown' in the review.

The calculated results for the $He^{2+} + Li$ system are presented in figure 2. Ionisation of one of the lithium atom K-shell electrons relative to the Li(2s) valence electron is a minor process (<1%) at 50 keV amu^{-1} but increases in importance and amounts to about 16% of the cross section at 400 keV amu^{-1}. The single electron capture process is primarily due to capture of a K-shell electron over most of the energy range. At 50 keV amu^{-1}, electron capture from the core is about 40% of the total cross section, but the K-shell capture contribution rises rapidly to around 90% at 100 keV amu^{-1} and is greater than 99% at 400 keV amu. The double electron capture cross section for $He^{2+} + Li$ is determined by the capture of both K-shell electrons

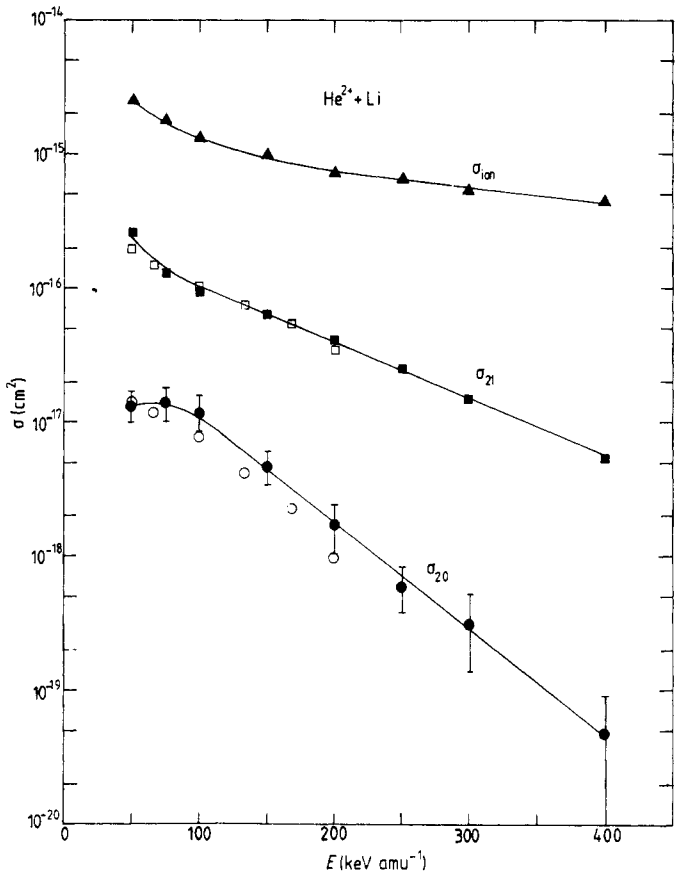

Figure 2. Calculated single electron capture, ionisation and double electron capture cross sections for the $He^{2+}+Li$ system: full squares, triangles, and circles, respectively. Experimental data from McCullough *et al* (1981) for the single and double electron capture processes are denoted by open squares and circles, respectively.

from the lithium atom. The error bars (2σ) on this cross section are statistical uncertainties that are attributable to the small number of trajectories that can lead to double electron capture even with the use of 10,000 trajectories at a given energy. Recently, McCullough *et al* (1981) measured the electron capture cross sections for the $He^{2+}+Li$ system. We have found good agreement with the experimental values for single capture, but our results lie almost a factor or two above the data for double capture at energies above 100 keV amu^{-1}.

Our estimated accuracy for the calculated single electron capture and ionisation cross sections is ±50%. The major uncertainty arises from the use of a hydrogenic model to represent the lithium atom shell structure. Thus, we are in disagreement with the $H^+ + Li$ experimental data for single electron capture. For the $He^{2+}+Li$ double electron capture process, our error estimate is much larger, being approximately a factor of three. This arises in part from the large statistical uncertainties for the double capture process that are shown in figure 2 and in part from the use of a hydrogenic model for the lithium atom. Our most serious uncertainty, however, arises from the application of the 'sudden' approximation in the IEM. To ascribe error limits,

we compared the calculations given in figure 2 with those for which sequential capture of the two electrons was assumed. These calculations reveal that our double electron capture results are uncertain by almost a factor of three. Therefore, the combination of statistical uncertainties and the uncertainty in the theoretical model limits us to an accuracy of approximately a factor of three for the double capture results. Thus, our calculations agree with the data of McCullough *et al* (1981).

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