Electron capture from hydrogen atoms by fast $Li^{+1}(1s^2)$, $Li^{+2}(1s)$, and Li^{+3} ions

K. E. Banyard and G. W. Shirtcliffe
Department of Physics, University of Leicester, Leicester LE1 7RH, England
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The continuum intermediate-states approximation has been used in the evaluation of cross sections for electron capture by $Li^{+1}(1s^2)$, $Li^{+2}(1s)$, and Li^{+3} ions from hydrogen atoms within an ionic energy range of 200 keV $\leq E \leq$ 10 000 keV. For each projectile system, the total capture cross sections were compared with the results of Shah, Goffe, and Gilbody [J. Phys. B 11, L233 (1978)] over a quoted experimental range 65 keV $\leq E \leq$ 1500 keV.

I. INTRODUCTION

Electron capture by lithium ions from hydrogen atoms in high-energy collisions has recently assumed some importance in the design and development of fusion reactors.[1,2] Thus charge-exchange cross sections $\sigma(nl)$ are reported here for the reactions

$$Li^{+q} + H(1s) \rightarrow Li^{+(q-1)}(nl) + H^+ , \quad (1)$$

where $q = 1$, 2, or 3 and the quantum numbers (nl) denote the final state of the "active" or captured electron. Since one objective of this work was to determine $\sigma(nl)$ at high relative velocities, the impact energy E for each lithium ion was allowed to vary from 200 to 10 000 keV. At the lower end of this energy range a q^3-scaling relationship between the cross sections has been examined in detail by Crothers and Todd.[3] For each ion, we evaluate the total cross section Q by invoking the Oppenheimer n^{-3} rule (see, for example, Salin[4]) and comparisons are made with experiment.

The cross sections are calculated by using the method of continuum intermediate states (CIS). The CIS approach, devised by Belkić[5] for electron capture by a structureless projectile, is closely related to the continuum distorted wave (CDW) method of Cheshire[6] but accounts for distortion effects in only one of the two channels. This feature enabled the method to be adapted previously for application to charge-exchange collisions between high-energy *structured* projectiles.[7] As an initial example, we studied the electron transfer between two hydrogen atoms. Consequently, our second objective is to use a similar scheme for reaction (1) when $q = 1$ and 2. For completeness, CIS results are also reported for $q = 3$ over the same energy range.

II. METHOD AND RESULTS

The cross section $\sigma(nl)$ for the capture of electron 1, say, by a fast projectile system of energy E in collision with a target (Z_B, e_1) considered to be at rest is written as

$$\sigma(nl) = 2\int_0^\infty b\,|a_{if}(b)|^2 db \ , \quad (2)$$

(in units of πa_0^2), where b is the impact parameter and a_{if} is the prior form of the transition amplitude. Atomic units are used throughout unless stated otherwise. For Li^{+3}, a_{if}, and hence $\sigma(nl)$, was determined by direct application of the CIS procedure. The bound-state wave functions and the energy decrement $\Delta\epsilon$ used in the method are exact since each electronic system is of hydrogenlike form. The capture cross sections for Li^{+3} striking hydrogen are given in Table I. The total cross-section Q was obtained from the n^{-3} rule

$$Q = \sigma(1s) + \sigma(2s) + \sigma(2p) + 2.081 \times [\sigma(3s) + \sigma(3p) + \sigma(3d)] \ . \quad (3)$$

The results are compared with the experimental data of Shah, Goffe, and Gilbody,[8] in Fig. 1, curve A.

For the structured projectile $Li^{+2}(1s)$, the modified form of the CIS method was used to determine $\sigma(nl)$. Following

TABLE I. Electron capture cross sections $\sigma(nl)$, measured in cm^2, for the reaction $Li^{+3} + H(1s) \rightarrow Li^{+2}(nl) + H^+$ at various impact energies E. The total cross section $Q = \sum_{(nl)} \sigma(nl)$ was evaluated by invoking the Oppenheimer n^{-3} rule. The superscript denotes the power of 10 by which each entry should be multiplied.

E (keV)	$\sigma(1s)$	$\sigma(2s)$	$\sigma(2p)$	$\sigma(3s)$	$\sigma(3p)$	$\sigma(3d)$	Q
200	1.0302×10^{-17}	9.1025×10^{-17}	7.6350×10^{-16}	9.1014×10^{-17}	5.4123×10^{-16}	1.2788×10^{-15}	4.8417×10^{-15}
500	2.7310×10^{-17}	1.4180×10^{-17}	6.8421×10^{-17}	1.3548×10^{-17}	3.0117×10^{-17}	1.2557×10^{-16}	4.6277×10^{-16}
1 000	5.7997×10^{-18}	1.9330×10^{-18}	1.0450×10^{-17}	1.0839×10^{-18}	4.5401×10^{-18}	9.7117×10^{-18}	5.0097×10^{-17}
2 000	6.2137×10^{-19}	1.6305×10^{-19}	9.7335×10^{-19}	5.8031×10^{-20}	4.5478×10^{-19}	3.0994×10^{-19}	3.4699×10^{-18}
5 000	2.7130×10^{-20}	7.9409×10^{-21}	1.2463×10^{-20}	2.8319×10^{-21}	5.2702×10^{-21}	1.0400×10^{-21}	6.6558×10^{-20}
10 000	1.7249×10^{-21}	3.7923×10^{-22}	2.2912×10^{-22}	1.2595×10^{-22}	8.9635×10^{-23}	7.8936×10^{-24}	2.7983×10^{-21}

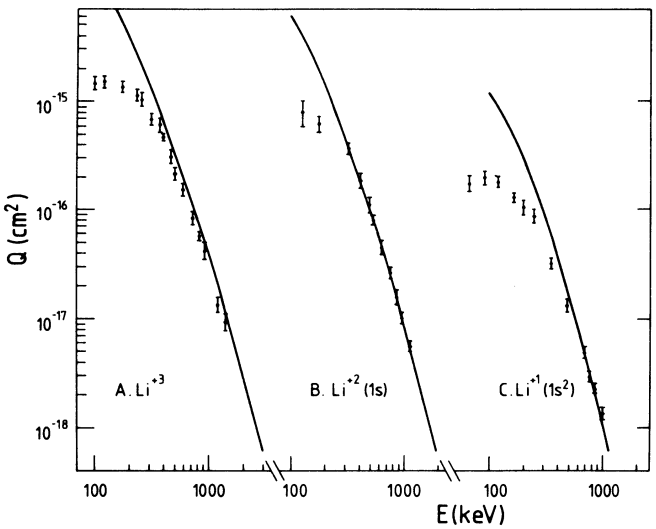

FIG. 1. Comparison of the total capture cross section Q with experiment (Ref. 8) when the projectile system is curve A, Li^{+3}; curve B, Li^{+2} (1*s*); and curve C, $Li^{+1}(1s^2)$.

our previous notation and approximations,[7] we may write

$$a_{if}=i\int_{-\infty}^{+\infty}\left\langle\Psi_f^-\left|\left(\frac{Z_A}{s_1}-\frac{1}{s_{12}}\right)\right|\chi_i\right\rangle dt\ , \qquad (4)$$

where Ψ_f^- is the final-state complete wave function and χ_i is the initial distorted wave. In the present calculation $Z_A=3$ and $Z_B=1$. As before, the interelectronic interaction was approximated by the average electrostatic potential arising from the orbital description of the passive electron within the projectile system. Hence, for $Li^{+2}(1s)$, the replacement

$$\left(\frac{Z_A}{s_1}-\frac{1}{s_{12}}\right)\rightarrow\frac{Z_A-1}{s_1}+\exp(-2Z_A s_1)\left(Z_A+\frac{1}{s_1}\right)\ , \qquad (5)$$

was made in Eq. (4) for a_{if}. The ground- and excited-capture states for $Li^{+}(1s,nl)$ were described, totally, by the Hartree-Fock (HF) treatment[9] and the "fixed core" results of Cohen and McEachran,[10,11] respectively. The capture cross sections are presented in Table II and the values for Q, obtained by use of Eq. (3), are compared with experiment in Fig. 1, curve B.

The evaluation of $\sigma(nl)$ for electron capture by $Li^{+1}(1s^2)$ followed the same general procedure as above. In the equivalent expression for a_{if} we made the replacement

$$\left(\sum_{i=1}^{2}\frac{Z_A}{s_i}-\sum_{\substack{i,j=1\\ i<j}}^{2}\frac{1}{s_{ij}}\right)\rightarrow\frac{(Z_A-2)}{s_1}+2\sum_k c_k e^{-2\xi_k s_1}\left(\xi_k+\frac{1}{s_1}\right)\ , \qquad (6)$$

where c_k and ξ_k are the coefficients and orbital exponents in the HF description of the passive electrons in the doubly occupied K shell of the Li^{+1} ion; $Z_A=3$ and $Z_B=1$ as above. An HF wave function[9] was used to describe $Li(1s^2,2s)$ whereas, for the excited states $Li(1s^2,nl)$, we generated our own functions by using a "fixed core" approximation, as discussed by Cohen and McEachran.[10,11] In this instance the "fixed core" is a completed K shell and was represented by the HF description taken from $Li(1s^2,2s)$. The excited orbitals were constructed from STO's (Slater-type orbitals) and mutual orthogonality was imposed on all the Li wave functions. The $\sigma(nl)$ values are given in Table III and a comparison of Q with experiment is shown in Fig. 1, curve C.

III. DISCUSSION

In addition to the results listed in Tables I–III, cross sections for each (nl) were calculated at several intermediate energies and the corresponding Q values were obtained but are not quoted here for reasons of space. Tables I and II indicate that $\sigma(1s)$ did not become the largest cross section until $E\gtrsim 3500$ keV. For all three reactions, we note that $\sigma(2l)>\sigma(3l)$ for each l.

The three sets of experimental data in Fig. 1 were taken from Shah, Goffe, and Gilbody[8] for a reported energy range of 65–1500 keV. Thus, the comparison between theory and experiment is rather limited since the CIS approach, like the CDW method, is essentially a high-velocity approximation; also, the use of the n^{-3} rule is probably incorrect in the lower-energy range. Consequently, it is not too surprising to observe that for each reaction the theoretical Q fails to reproduce the experimental results at low energies. However, for Li^{+3} and $Li^{+2}(1s)$, it was found that $\sigma(1s)$ did show the same characteristics in shape as experiment by falling away in magnitude as E was decreased below 400 and 250

TABLE II. Electron capture cross sections $\sigma(nl)$, measured in cm^2, for the reaction $Li^{+2}(1s)+H(1s)\rightarrow Li^{+1}(1s,nl)+H^{+}$ at various E. The total cross section is represented by Q. The superscript denotes the power of 10 by which each entry should be multiplied.

E (keV)	$\sigma(1s)$	$\sigma(2s)$	$\sigma(2p)$	$\sigma(3s)$	$\sigma(3p)$	$\sigma(3d)$	Q
200	3.2312×10^{-17}	6.3897×10^{-17}	4.0707×10^{-16}	5.6424×10^{-17}	1.8920×10^{-16}	1.8469×10^{-16}	1.3987×10^{-15}
500	7.9093×10^{-18}	4.0108×10^{-18}	4.0912×10^{-17}	2.1234×10^{-18}	1.4256×10^{-17}	4.5157×10^{-18}	9.6315×10^{-17}
1000	1.0952×10^{-18}	2.7473×10^{-19}	3.9405×10^{-18}	9.5591×10^{-20}	1.7233×10^{-18}	2.2532×10^{-19}	9.5645×10^{-18}
2000	1.2959×10^{-19}	3.6311×10^{-20}	2.2395×10^{-19}	1.2365×10^{-20}	9.0542×10^{-20}	1.7875×10^{-20}	6.4120×10^{-19}
5000	5.5768×10^{-21}	1.2846×10^{-21}	3.5101×10^{-21}	4.0230×10^{-22}	1.2478×10^{-21}	1.0898×10^{-21}	1.6073×10^{-20}
10000	3.0424×10^{-22}	5.4929×10^{-23}	1.4806×10^{-22}	1.6260×10^{-23}	4.8408×10^{-23}	1.1326×10^{-22}	8.7749×10^{-22}

TABLE III. Electron capture cross sections $\sigma(nl)$, measured in cm^2, for the reaction $Li^{+1}(1s^2) + H(1s) \rightarrow Li(1s^2,nl) + H^+$ at various E. The total cross section is represented by Q. The superscript denotes the power of 10 by which each entry should be multiplied.

E (keV)	$\sigma(2s)$	$\sigma(2p)$	$\sigma(3s)$	$\sigma(3p)$	$\sigma(3d)$	Q
200	1.4923×10^{-17}	1.1796×10^{-16}	7.3251×10^{-18}	7.3881×10^{-17}	6.2812×10^{-18}	3.1494×10^{-15}
500	1.7582×10^{-18}	5.2159×10^{-18}	9.5825×10^{-19}	3.6575×10^{-18}	2.0863×10^{-19}	1.7014×10^{-17}
1 000	2.8796×10^{-19}	2.2221×10^{-19}	1.3770×10^{-19}	1.6167×10^{-19}	5.2592×10^{-21}	1.1441×10^{-18}
2 000	2.8702×10^{-20}	5.6118×10^{-21}	1.2063×10^{-20}	4.1444×10^{-21}	6.6965×10^{-23}	6.8180×10^{-20}
5 000	7.0801×10^{-22}	2.8930×10^{-23}	2.6715×10^{-22}	2.1378×10^{-23}	1.1853×10^{-25}	1.3376×10^{-21}
10 000	3.0797×10^{-23}	4.9977×10^{-25}	1.1110×10^{-23}	3.6779×10^{-25}	9.1724×10^{-28}	5.5184×10^{-23}

keV, respectively. Nevertheless, the steady increase in cross section for capture into each excited state, for decreasing E, masks this $\sigma(1s)$ characteristic when evaluating Q. As E is increased, Fig. 1 shows that some agreement exists between theory and experiment for Q for each projectile. The best graphical agreement occurs for $Li^{+2}(1s)$ when $E \geqslant 300$ keV. For Li^{+3}, it should be noted that the size of the charge on the projectile makes it a somewhat severe example for the prior form of the CIS method.

Finally, for the structured projectiles $Li^{+2}(1s)$ and $Li^{+1}(1s^2)$, the present relation between theory and experiment shows a quite noticeable improvement over that obtained from our earlier calculation[7] on the test reaction $H(1s) + H(1s) \rightarrow H^-(1s^2) + H^+$.

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