Laser-enhanced Ly α emission from H⁺Li(2p_m) collisions

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Abstract

Li(2s,2p)-H⁺ charge transfer is studied using an eight adiabatic molecular basis and the impact parameter method with a common translation factor in the range 0.5–10 keV. The Ly α enhancement for capture to H(2p) from excited Li(2p) and orientation preference from Li (2p₋₁) is obtained.

Introduction

Investigations of charge transfer collisions between singly or multiply charged ionic projectiles and neutral atoms has, up to now, been concentrated on target atoms in spherically symmetric ground states. At present, tunable dye lasers are a very good tool for preparation of target atoms in specific excited states with a concrete alignment and orientation [1]. A prototype reaction for such studies is

The electron capture process from Na atoms in the ground state has been extensively studied theoretically [2] and experimentally [3] because of a long disagreement between these two kinds of results. The conclusions are: (i) an enhancement of Ly α radiation after the collision at low energies when the initial state is Na^{*}(3p); (ii) if the initial state is circularly polarized Na^{*}(3p) (prepared with a dye laser beam), the capture cross section is bigger when the electron in the initial orbit has an angular velocity in the same sense as the incident proton (3p₋₁).

Another prototype of a quasi-one-electron system is the collision

which has been studied in the past for the total capture cross sections only from the ground state (Li(2s)) [4]. Reaction (2) is interesting for the following reasons:

- (i) It is a very simple system for the testing ground and excited theoretical descriptions of capture processes for quasi-resonant systems;
- (ii) determination of laser enhancement Ly α emission from the capture process at low energies;
- (iii) such processes are of interest for fusion plasma diagnostics [5].

In this paper we are interested in the theoretical treatment for electron capture processes involving aligned and oriented electronic states for the target atom Li(2s,2p_m) in the energy range $0.5 < E_{\text{cm}} < 10$ keV. The total and partial cross sections and probabilities are presented for this collision system.

Theoretical model

Model potential and molecular states

We use a particular form of model potential

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successful in previous applications in atomic collisions [6]

$$V(r) = -\frac{1}{r} - \frac{2}{r}(1 + \alpha r) \exp(-\beta r)$$

where $\alpha = 1.655$ and $\beta = 3.31$.

This form guarantees correct long and short range limits. The parameters α and β are fitted to reproduce the experimental atomic energy levels accurately. The basis set used to calculate the atomic eigenvalues of the one-electron hamiltonian are Slater-type orbitals in prolate spheroidal coordinates with foci on the nuclei. With this basis we build the eight molecular states functions minimum to reproduce the electron capture to $H^*(n=2)$: $2^2\Sigma(2s\sigma\text{Li})$, $3^2\Sigma(2p\sigma\text{Li})$, $1^2\Pi(2p\pi^\pm\text{Li})$, $2^2\Pi(2p\pi^\pm\text{H})$, $4^2\Sigma(\phi^+\text{H})$ and $5^2\Sigma(\phi^-\text{H})$. The two last states correspond to the Stark split states. The atomic limit of each molecular state is in parentheses. The labels “+” and “-” refer to the symmetry of the molecular state is respect to the reflection in the collision plane.

These molecular states are used to calculate the radial and rotational matrix elements necessary in the dynamical description.

Dynamical model

The coupled differential equations which we use

to find the transition amplitudes in the collision problem are derived from the time-dependent Schrödinger equation. The impact parameter approximation is valid in the energy range studied (0.5–10 keV) with the inclusion of a common translation factor (CTF) [7]

$$U(r, R) = f(r, R)v \cdot r - \frac{1}{2}f^2(r, R)v^2 t$$

$$f(r, R) = \hat{R} \cdot r / R$$

to take into account the electron transfer momentum problem. The Stark effect at long distance, which induces a large coupling between H^* (2s) and H^* (2p), is included in the evolution matrix U in order to find the correct final state distribution flux in $H^*(n=2)$. The coupled equations are solved up to $z_0 = 30$ a.u. for each impact parameter and the final amplitudes $a(+\infty)$ are obtained by [2]

$$a_m(+\infty) = U(z_0, +\infty)a_m(z_0)$$

Couplings

The radial and rotational couplings include the terms coming from the CTF corrections to first order in the relative velocity of the two nuclei.

Fig. 1. Total capture cross section ($\text{\AA}^2$) vs. energy (keV). (a) Li(2s), to $H(n=2)$: —, present results; ---, Fritsch; - x -, Ermolaev; *, Aumayr; □, Varghese [4]. (b) Present results: ---, Li(2p) to H(2p); - x - Li(2s) to H(2p); —, Li(2p)/Li(2s) to H(2p); *, Li(2s) to H(2p) (experimental values, Aumayr [4]).

In the $\text{Li}-\text{H}^+$ system, the most important couplings we found for interpretation of electronic capture to $\text{H}^*(n=2)$ are as follows.

From $\text{Li}(2s)$

$\langle 2^2\Sigma|\partial/\partial R|3^2\Sigma\rangle$ has a maximum at $R \approx 11$ a.u. corresponding to the avoided crossing that provides a direct mechanism for excitation to $\text{Li}^*(2p)$, followed by $\langle 3^2\Sigma|i\text{Ly}|2^2\Pi\rangle$ coupling, to account for the electronic capture to $\text{H}^*(2p\pi)$. This is important at large range (5–25 a.u.). The coupling $\langle 2^2\Sigma|i\text{Ly}|2^2\Pi\rangle$ has a peak at $R \approx 5$ a.u. and provides a direct mechanism for electronic capture at short distance.

From $\text{Li}^(2p)$*

Coupling $\langle 3^2\Sigma|i\text{Ly}|2^2\Pi\rangle$ (as explained before), $\langle 3^2\Sigma|\partial/\partial R|4^2\Sigma\rangle$ with a peak at $R \approx 25$ a.u. and $\langle 1^2\Pi|i\text{Ly}|5^2\Sigma\rangle$ with a peak at $R \approx 10$ a.u. are responsible for this transition.

These couplings, similar to those obtained by Sato and Kimura [8] with an atomic basis, explain the main features for electronic capture.

Results

Total and partial cross sections

We have calculated the total and partial cross sections for the following electronic capture processes.

Process a

Process b

Process b is expected to be dominant because the value of ΔE_b reflects quasi-resonant energy levels.

Comparison of capture cross sections from $\text{Li}(2s)$ with other results are shown in Fig. 1(a). Our results compare fairly well in the range 0.5–6 keV, where the enhancement is important. At higher energies there is a disagreement for the $\text{Li}(2s)$ to $\text{H}^*(n=2)$ transition. We expect to explain it by including higher excited states to allow a better description of the electronic flux at higher energies. In this range of energies the capture into $\text{H}^*(2p)$ (Fig. 1(b)) is more important from $\text{Li}^*(2p)$ than from $\text{Li}(2s)$. This establishes an enhancement of $\text{Ly}\alpha$ radiation when the initial state is the former. This great increase at low energies in the cross sections reflects the quasi-resonance $\text{Li}^*(2p)-\text{H}^*(2p)$ energy states.

Orientation

Using a laser beam with circularly polarized light, it is possible to prepare a $\text{Li}^*(2p_{\pm 1})$ oriented state and to study the influence of this orientation in the total electron cross section to $\text{H}^*(2p)$.

From a theoretical point of view we change the molecular basis to the atomic basis functions in the incoming channels by

$$\begin{bmatrix} |2p_0\rangle \\ |2p_{+1}\rangle \\ |2p_{-1}\rangle \end{bmatrix}^{XYZ} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & \sqrt{2} \\ 1 & -i & 0 \\ -1 & -i & 0 \end{bmatrix} \begin{bmatrix} |2p_\sigma\rangle \\ |2p_{\pi^+}\rangle \\ |2p_{\pi^-}\rangle \end{bmatrix}^{xyz}$$

The XYZ frame is the laboratory fixed frame and xyz is the molecular frame. It is necessary to take into account that if $t \rightarrow -\infty$, we must change the orientation of the molecular axis frame with respect to the laboratory frame because of the relative rotation.

Figure 2(a) shows the probabilities for the capture to $\text{H}^*(2p)$ from $\text{Li}^*(2p_{\pm 1})$ at 2 keV. It is clear from Fig. 2(a) that at this energy the capture from the oriented $\text{Li}^*(2p_{-1})$ state is also dominant at large impact parameter, similarly to the $\text{Na}-\text{H}^+$ case [2]. From a classical point of view, this fact corresponds to the proton having a

Fig. 2. Capture probability involving oriented states: (a) —, $\text{Li}(2p_{-1})$ to $\text{H}(2p)$; ---, $\text{Li}(2p_{+1})$ to $\text{H}(2p)$. (b) $\text{Li}(2p_{-1})$ to $\text{H}(2p_{-1})$.

velocity in the same sense as the electron in the $\text{Li}^*(2p_{-1})$ atom.

Further, we also analyzed both the initial and final oriented states capture in order to explain the velocity matching rule. The capture probabilities show (Fig. 2(b)) a preference when the electron has an angular velocity in the same sense as the incident proton. The maximum probability is reached at 0.45 a.u. (very close to the classical value for the electron velocity in the $\text{Li}^*(2p)$).

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