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# Theory and application of hydrogen formation in proton-alkali atom collision 

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#### Abstract

The possibility of producing more hydrogen during p-alkali atom collisions is discussed. The coupled static approximation is modified for the first time to make it applicable to the multichannel problem of the collisions of p-alkali atoms. The formation of $\mathrm{H}(1 \mathrm{~s})$ and excited H (in $2 \mathrm{~s}-$ and 2 p - states) in the scattering of p -Li atoms is treated to test the convergence of our method. The modified method is used to calculate the total cross-sections of seven partial waves in a range of energy between 50 and 1000 keV . Our p-Li results are compared with earlier ones.


Key words: Proton-alkali, hydrogen formation, excited hydrogen formation, cross-sections

## 1. Introduction

The most interesting phenomenon in quantum mechanics is the intermediate states that appear in a nuclear reaction. Most theoretical and experimental studies of proton-atom interactions have been discussed in the last decade by many authors. They calculated the total cross-sections of the interaction. Banyard and Shirtcliffe [1] discussed p-Li scattering using continuum distorted wave (CDW) approximation. Ferrante and Fiordilino [2] studied p-alkali atoms using eikonal approximations. Daniele et al. [3] reported the total cross-sections for p-alkali atom collision using eikonal approximation. Ferrante et al. [4] also investigated the total H-formation cross-sections in p-alkali atoms using Oppenheimer-Brinkman-Kramers (OBK) approximation. Fritsch and Lin [5] studied p-H atom collisions using the coupled-state calculations method. Choudhury and Sural [6] studied p-alkali atom ( $\mathrm{Na}, \mathrm{K}, \mathrm{Rb}, \mathrm{Cs}$ ) collisions in the wave formation of impulse approximation at energies ranging from 50 to 500 keV . Tiwari [7] reported the differential and total cross-sections in H-formation in the collision of $\mathrm{p}-\mathrm{Li}$ and $\mathrm{p}-\mathrm{Na}$ atoms using Coulomb-projected Born approximation.

The present work explores the possibility of producing more hydrogen through p-alkali atom collisions. In the present paper, the coupled static approximation (CSA) method, which is used by Elkilany [8-11], is modified to make it applicable to discuss the multichannel coupled static approximation (MCSA) problem ( $n=$ 4) of the collision of $\mathrm{p}-\mathrm{Li}$ atoms at intermediate energies of the projectile. A numerical procedure is generalized to solve the obtained multicoupled equations. Throughout this paper Rydberg units are used and the total cross-sections are expressed in units of $\pi a_{0}^{2}\left(=8.8 \times 10^{-17} \mathrm{~cm}^{2}\right)$ and energy units of keV .

## 2. Theoretical formalism

The MCSA of protons scattered by alkali atoms may be written as (see Figure 1):

[^0]

Figure 1. Configuration space of p-atom scattering: $\bar{x}_{i}$ and $\bar{r}_{i}$ are the vectors of the proton and the valence electron of the target with respect to the center of mass of the target, $\bar{\rho}_{i}$ is the vector of the proton with respect to the valence electron of the target, $\bar{\sigma}_{i}$ is the vector of the center of mass of $H$ from the target, and $M_{T}$ is the mass of the nucleus of the target.

$$
p+A=\left[\begin{array}{ll}
p+A & \text { Elastic channel ( first channel) }  \tag{1}\\
H(n \ell)+A^{+} & H(n \ell) \text { formation channels }((n-1)-\text { channels })
\end{array},\right.
$$

where $p$ is the proton, $A$ is an alkali target atom, $H(n \ell)$ is hydrogen formation in $n \ell$-states, and $n$ is the number of open channels.

The Hamiltonian of the elastic channel is given by:

$$
\begin{equation*}
H=H^{(1)}=H_{T}-\frac{1}{2 \mu_{1}} \nabla_{x_{1}}^{2}+V_{i n t}^{(1)}\left(x_{1}\right)=-\frac{1}{2 \mu_{T}} \nabla_{r_{1}}^{2}-\frac{2}{r_{1}}+V_{c}\left(r_{1}\right)-\frac{1}{2 \mu_{1}} \nabla_{x_{1}}^{2}+V_{i n t}^{(1)}\left(x_{1}\right), \tag{2}
\end{equation*}
$$

where $H_{T}$ is the Hamiltonian of the target atom. $\mu_{T}$ is the reduced mass of the target atom.

$$
\begin{equation*}
H=H^{(i)}=H_{i}-\frac{1}{2 \mu_{i}} \nabla_{\sigma_{i}}^{2}+V_{i n t}^{(i)}\left(\sigma_{i}\right)=-\frac{1}{2 \mu_{i}} \nabla_{\rho_{i}}^{2}-\frac{2}{\rho_{i}}-\frac{1}{2 \mu_{i}} \nabla_{\sigma_{i}}^{2}+V_{i n t}^{(i)}\left(\sigma_{i}\right), i=2,3,4, \ldots n \tag{3}
\end{equation*}
$$

The Hamiltonian of the ( $n-1$ )-rearrangement channels are expressed by:
Here, $H_{i}, i=2,3,4, \ldots n$ are the Hamiltonians of the hydrogen formation atoms, $H(n l)$, respectively. $\mu_{i}, i=2,3,4, \ldots n$ are the reduced masses of $(n-1)-$ channels, respectively.
$V_{c}\left(r_{1}\right)$ is a screened potential and $V_{i n t}^{(1)}\left(x_{1}\right)$ is the interaction potential of the first channel, given by:

$$
\begin{equation*}
V_{c}\left(r_{1}\right)=V_{c \operatorname{Coul}}\left(r_{1}\right)+V_{c e x}\left(r_{1}\right) \tag{4}
\end{equation*}
$$

where $V_{c C o u l}\left(r_{1}\right)$ and $V_{\text {cex }}\left(r_{1}\right)$ are the Coulomb and exchange parts of the core potential, respectively (see ref. [11]), and

$$
\begin{equation*}
V_{i n t}^{(1)}\left(x_{1}\right)=\frac{2}{x_{1}}-\frac{2}{\rho_{1}}+V_{c C o u l}\left(x_{1}\right) \text { where } V_{c C o u l}\left(x_{1}\right)=-V_{c C o u l}\left(r_{1}\right) \tag{5}
\end{equation*}
$$

and $V_{i n t}^{(i)}\left(\sigma_{i}\right)$, is the interaction between the two particles of the considered hydrogen formation and the rest of the target, which is given by:

$$
\begin{equation*}
V_{i n t}^{(i)}\left(\sigma_{i}\right)=\frac{2}{x_{i}}-\frac{2}{r_{i}}+V_{c C o u l}\left(x_{i}\right)+V_{c C o u l}\left(r_{i}\right)+V_{c e x}\left(r_{i}\right), i=2,3,4, \ldots n \tag{6}
\end{equation*}
$$

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The total energies $E$ of the $n$-channels are defined by:

$$
\begin{equation*}
E=E_{i}+\frac{1}{2 \mu_{i}} k_{i}^{2}, i=1,2,3 \ldots n \tag{7}
\end{equation*}
$$

where $\frac{1}{2 \mu_{1}} k_{1}^{2}$ is the kinetic energy of the incident proton relative to the target and $\frac{1}{2 \mu_{i}} k_{i}^{2}, i=2,3,4, \ldots, n$ are the kinetic energy of the center of mass of the hydrogen formation atoms, $H(n \ell)$, respectively, relative to the nucleus of the target. $E_{1}$ is the binding energy of the target atom, and $E_{i}, i=2,3,4, \ldots, n$ refer to the binding energies of the hydrogen formation atoms, respectively.

In MCSA, it is assumed that the projections of the vector $(H-E)|\Psi\rangle$ onto the bound state of the $n$-channels are zero. Thus, the following conditions are satisfied:

$$
\begin{equation*}
\left\langle\Phi_{i}\right|(H-E)|\Psi\rangle=0, i=1,2,3, \ldots, n \tag{8}
\end{equation*}
$$

The total wave function $|\Psi\rangle$ is expressed by

$$
\begin{gather*}
\Psi=\sum_{i=1}^{n}\left|\phi_{i} \psi_{i}\right\rangle,  \tag{9}\\
\psi_{1}=\sum_{\ell} \ell(\ell+1) f_{\ell}^{(1)}\left(x_{1}\right) Y_{\ell}^{0}\left(\hat{x}_{1}\right),  \tag{10}\\
\psi_{i}=\sum_{\ell} \ell(\ell+1) g_{\ell}^{(i)}\left(\sigma_{i}\right) Y_{\ell}^{0}\left(\hat{\sigma}_{i}\right), i=2,3, \ldots n \tag{11}
\end{gather*}
$$

where $f_{\ell}^{(1)}\left(x_{1}\right)$ and $g_{\ell}^{(i)}\left(\sigma_{i}\right), i=2,3, \ldots n$ are the radial wave functions of the elastic and the hydrogen formation atoms, respectively, corresponding to the total angular momentum $\ell . Y_{\ell}^{0}\left(x_{1}\right)$ and $Y_{\ell}^{0}\left(\hat{\sigma}_{i}\right) i=2,3, \ldots, n$ are the related spherical harmonics. $\hat{x}_{1}$ and $\hat{\sigma}_{i}, i=1,2,3, \ldots, n$ are the solid angles between the vectors $\hat{x}_{1}, \hat{\sigma}_{i}, i=$ $2,3, \ldots n$ and the z-axis, respectively. $\psi_{i}, i=1,2,3, \ldots n$ are the corresponding scattering wave functions of the $n$-channels, respectively. $\Phi_{1}$ is the wave function for the valence electron of the target atom, which is calculated using ref. [12]. $\Phi_{i}, i=2,3,4, \ldots, n$ are the wave functions of the hydrogen formation atoms, $H(n \ell)$, respectively, which are defined using a hydrogen-like wave function.

Eq. (8) can be solved by considering differential equations

$$
\begin{gather*}
{\left[\frac{d^{2}}{d x_{1}^{2}}-\frac{\ell(\ell+1)}{x_{1}^{2}}+k_{1}^{2}\right] f_{\ell}^{(1)}\left(x_{1}\right)=2 \mu_{1} U_{s t}^{(1)}\left(x_{1}\right) f_{\ell}^{(1)}\left(x_{1}\right)+\sum_{\alpha=2}^{n} Q_{1 \alpha}\left(x_{1}\right),}  \tag{12}\\
{\left[\frac{d^{2}}{d \sigma_{i}^{2}}-\frac{\ell(\ell+1)}{\sigma_{i}^{2}}+k_{i}^{2}\right] g_{\ell}^{(i)}\left(\sigma_{i}\right)=2 \mu_{i} U_{s t}^{(i)}\left(\sigma_{i}\right) g_{\ell}^{(i)}\left(\sigma_{i}\right)+\sum_{\alpha=1}^{n} Q_{i \alpha}\left(\sigma_{i}\right), i=2,3, \ldots, n,} \tag{13}
\end{gather*}
$$

where the prime on the sum sign means that $i \neq \alpha$, and

$$
\begin{equation*}
Q_{1 \alpha}\left(x_{1}\right)=\int_{0}^{\infty} K_{1 \alpha}\left(x_{1}, \sigma_{\alpha}\right) g_{\ell}^{(\alpha)}\left(\sigma_{\alpha}\right) d \sigma_{\alpha}, \alpha=2,3, \ldots, n \tag{14}
\end{equation*}
$$

$$
\begin{gather*}
Q_{i 1}\left(\sigma_{i}\right)=\int_{0}^{\infty} K_{i 1}\left(\sigma_{i}, x_{1}\right) f_{\ell}^{(1)}\left(x_{1}\right) d x_{1}, i=2,3, \ldots, n  \tag{15}\\
Q_{i \alpha}\left(\sigma_{i}\right)=\int_{0}^{\infty} K_{i \alpha}\left(\sigma_{i}, \sigma_{\alpha}\right) g_{\ell}^{(\alpha)}\left(\sigma_{\alpha}\right) d \sigma_{\alpha}, i, \alpha=2,3, \ldots, n, i \neq \alpha . \tag{16}
\end{gather*}
$$

Kernels $K_{i \alpha}, i=1,2,3, \ldots, n, i \neq \alpha$ are expanded by:

$$
\begin{align*}
& K_{1 \alpha}\left(x_{1}, \sigma_{\alpha}\right)=2 \mu_{1}\left(8 x_{1} \sigma_{\alpha}\right) \iint \Phi_{1}\left(r_{1}\right) \Phi_{\alpha}\left(\rho_{\alpha}\right)\left[-\frac{1}{2 \mu_{\alpha}}\left(\nabla_{\sigma_{\alpha}}^{2}+k_{\alpha}^{2}\right)+V_{i n t}^{(\alpha)}\right] Y_{\ell}^{o}\left(\hat{x}_{1}\right) Y_{\ell}^{o}\left(\hat{\sigma}_{\alpha}\right) d \hat{x}_{1} d \hat{\sigma}_{\alpha}  \tag{17}\\
& \alpha=2,3, \ldots n \\
& K_{i 1}\left(\sigma_{i}, x_{1}\right)=2 \mu_{i}\left(8 \sigma_{i} x_{1}\right) \iint \Phi_{i}\left(\rho_{i}\right) \Phi_{1}\left(r_{1}\right)\left[-\frac{1}{2 \mu_{1}}\left(\nabla_{x_{1}}^{2}+k_{1}^{2}\right)+V_{i n t}^{(1)}\right] Y_{\ell}^{o}\left(\hat{\sigma}_{i}\right) Y_{\ell}^{o}\left(\hat{x}_{1}\right) d \hat{\sigma}_{i} d \hat{x}_{1}, i=2,3, \ldots n  \tag{18}\\
& K_{i \alpha}\left(\sigma_{i}, \sigma_{\alpha}\right)=  \tag{19}\\
& 2 \mu_{i}\left(8 \sigma_{i} \alpha_{\alpha}\right) \iint \Phi_{i}\left(\rho_{i}\right) \Phi_{\alpha}\left(\rho_{\alpha}\right)\left[-\frac{1}{2 \mu_{\alpha}}\left(\nabla_{\sigma_{\alpha}}^{2}+k_{\alpha}^{2}\right)+V_{i n t}^{(\alpha)}\right] Y_{\ell}^{o}\left(\hat{\sigma}_{i}\right) Y_{\ell}^{o}\left(\hat{\sigma}_{\alpha}\right) d \hat{\sigma}_{i} d \hat{\sigma}_{\alpha} \\
& \\
& i, \alpha=2,3, \ldots n, i \neq \alpha
\end{align*}
$$

The static potentials $U_{s t}^{(1)}\left(x_{1}\right)$ and $U_{s t}^{(i)}\left(\sigma_{i}\right), i=2,3, \ldots, n$ are defined by

$$
\begin{equation*}
U_{s t}^{(1)}\left(x_{1}\right)=<\Phi_{1}\left(r_{1}\right)\left|V_{i n t}^{(1)}\right| \Phi_{1}\left(r_{1}\right)>, \quad U_{s t}^{(i)}\left(\sigma_{i}\right)=<\Phi_{i}\left(\rho_{i}\right)\left|V_{i n t}^{(i)}\right| \Phi_{i}\left(\rho_{i}\right)> \tag{20}
\end{equation*}
$$

Eqs. (12) and (13) are inhomogeneous equations in $x_{i}$, and $\sigma_{i}, i=1,2,3, \ldots, n$, and possess the general form

$$
\begin{equation*}
\left.\left(\varepsilon-H_{0}\right)|\chi>=| \eta\right\rangle \tag{21}
\end{equation*}
$$

where $\varepsilon$ is $k_{i}^{2}(i=1,2, \ldots, n) . \quad H_{0}$ is $-\frac{d^{2}}{d x_{1}^{2}}+\frac{\ell(\ell+1)}{x_{1}^{2}}$ or $-\frac{d^{2}}{d \sigma_{i}^{2}}+\frac{\ell(\ell+1)}{\sigma_{i}^{2}}, i=2,3, \ldots, n .|\chi\rangle$ is $\left|f_{\ell}^{(1)}\left(x_{1}\right)\right\rangle$ or $\left|g_{\ell}^{(i)}\left(\sigma_{i}\right)\right\rangle .|\eta\rangle$ is the right-hand side of the coupled integro-differential equations, respectively.

The solutions of Eqs. (12) and (13) are given (formally) by the Lippmann-Schwinger equation in the form

$$
\begin{equation*}
\left|\chi>=\left|\chi_{o}>+G_{o}\right| \eta>\right. \tag{22}
\end{equation*}
$$

where $G_{0}$ is the Green operator $\left(\varepsilon-H_{0}\right)^{-1}$ and $\left|\chi_{0}\right\rangle$ is the solution of the homogeneous equation

$$
\begin{equation*}
\left(\varepsilon-H_{0}\right)\left|\chi_{0}\right\rangle=|0\rangle, \tag{23}
\end{equation*}
$$

Using Green operator $G_{0}$, the solutions of Eqs. (12) and (13) are given formally by

$$
\begin{align*}
f_{\ell}^{(1, j)}\left(x_{1}\right)= & \left\{\delta_{j 1}+\frac{1}{k_{1}} \int_{0}^{\infty} \tilde{g}_{\ell}\left(k_{1} x_{1}\right)\left[2 \mu_{1} U_{s t}^{(1)}\left(x_{1}\right) f_{\ell}^{(1, j)}\left(x_{1}\right)+\sum_{\alpha=2}^{n} Q_{1 \alpha}^{(j)}\left(x_{1}\right)\right] d x_{1}\right\} \tilde{f}_{\ell}\left(k_{1} x_{1}\right) \\
& +\left\{-\frac{1}{k_{1}} \int_{0}^{\infty} \tilde{f}_{\ell}\left(k_{1} x_{1}\right)\left[2 \mu_{1} U_{s t}^{(1)}\left(x_{1}\right) f_{\ell}^{(1, j)}\left(x_{1}\right)+\sum_{\alpha=2}^{n} Q_{1 \alpha}^{(j)}\left(x_{1}\right)\right] d x_{1}\right\} \tilde{g}_{\ell}\left(k_{1} x_{1}\right), j=1,2,3, \ldots, n \tag{24}
\end{align*}
$$

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$$
\begin{align*}
g_{\ell}^{(i, j)}\left(\sigma_{i}\right)= & \left\{\delta_{j i}+\frac{1}{k_{i}} \int_{0}^{\infty} \tilde{g}_{\ell}\left(k_{i} \sigma_{i}\right)\left[2 \mu_{i} U_{s t}^{(i)}\left(\sigma_{i}\right) g_{\ell}^{(i, j)}\left(\sigma_{i}\right)+\sum_{\alpha=1}^{n} Q_{i \alpha}\left(\sigma_{i}\right)\right] d \sigma_{i}\right\} \tilde{f}_{\ell}\left(k_{i} \sigma_{i}\right) \\
& +\left\{-\frac{1}{k_{i}} \int_{0}^{\infty} \tilde{f}_{\ell}\left(k_{i} \sigma_{i}\right)\left[2 \mu_{i}{\underset{s t}{U}}_{(i)}^{\left(\sigma_{i}\right)} g_{\ell}^{(i, j)}\left(\sigma_{i}\right)+\sum_{\alpha=1}^{n} Q_{i \alpha}^{(j)}\left(\sigma_{i}\right)\right] d \sigma_{i}\right\} \tilde{g}_{\ell}\left(k_{i} \sigma_{i}\right),  \tag{25}\\
& i=2,3, \ldots, n \quad j=1,2,3, \ldots, n
\end{align*}
$$

where $\delta_{j i}, i, j=1,2,3, \ldots, n$ specify two independent solutions for each of $f_{\ell}^{(1, j)}\left(x_{1}\right)$ and $g_{\ell}^{(i, j)}\left(\sigma_{i}\right), i=2,3, \ldots, n$, according to the considered channel. The functions $\tilde{f}_{l}(\eta)$ and $\tilde{g}_{l}(\eta), \eta=k_{1} x_{1}$, or $\eta=k_{i} \sigma_{i} i=2,3, \ldots, n$ are related to the Bessel functions of the first and second kinds, i.e. $j_{l}(\eta)$ and $y_{l}(\eta)$, respectively, by the relations $\tilde{f}_{l}(\eta)=\eta j_{l}(\eta)$ and $\tilde{g}_{l}(\eta)=-m y_{l}(\eta)$.

The iterative solutions of Eqs. (24) and (25) are calculated by:

$$
\begin{align*}
f_{\ell}^{(1, j, \nu)}\left(x_{1}\right)= & \left\{\delta_{j 1}+\frac{1}{k_{1}} \int_{0}^{x_{1}} \tilde{g}_{\ell}\left(k_{1} x_{1}\right)\left[2 \mu_{1} U_{s t}^{(1)}\left(x_{1}\right) f_{\ell}^{(1, j, \nu-1)}\left(x_{1}\right)+\sum_{\alpha=2}^{n} Q_{1 \alpha}^{(j, \nu-1)}\left(x_{1}\right)\right] d x_{1}\right\} \tilde{f}_{\ell}\left(k_{1} x_{1}\right) \\
& +\left\{-\frac{1}{k_{1}} \int_{0}^{X_{1}} \tilde{f}_{\ell}\left(k_{1} x_{1}\right)\left[2 \mu_{1} U_{s t}^{(1)}\left(x_{1}\right) f_{\ell}^{(1, j, \nu-1)}\left(x_{1}\right)+\sum_{\alpha=2}^{n} Q_{1 \alpha}^{(j, \nu-1)}\left(x_{1}\right)\right] d x_{1}\right\} \tilde{g}_{\ell}\left(k_{1} x_{1}\right),  \tag{26}\\
j= & 1,2,3, \ldots, n ; \nu \geq 1 . \\
g_{\ell}^{(i, j, \nu)}\left(\sigma_{i}\right)= & \left\{\delta_{j i}+\frac{1}{k_{i}} \int_{0}^{\sum_{i}} \tilde{g}_{\ell}\left(k_{i} \sigma_{i}\right)\left[2 \mu_{i} U_{s t}^{(i)}\left(\sigma_{i}\right) g_{\ell}^{(i, j, \nu)}\left(\sigma_{i}\right)+\sum_{\alpha=1}^{n} Q_{i \alpha}^{(j, \nu)}\left(\sigma_{i}\right)\right] d \sigma_{i}\right\} \tilde{f}_{\ell}\left(k_{i} \sigma_{i}\right) \\
& +\left\{-\frac{1}{k_{i}} \int_{0}^{\sum_{i}} \tilde{f}_{\ell}\left(k_{i} \sigma_{i}\right)\left[2 \mu_{i} U_{s t}^{(i)}\left(\sigma_{i}\right) g_{\ell}^{(i, j, \nu)}\left(\sigma_{i}\right)+\sum_{\alpha=1}^{n} Q_{i \alpha}^{(j, \nu)}\left(\sigma_{i}\right)\right] d \sigma_{i}\right\} \tilde{g}_{\ell}\left(k_{i} \sigma_{i}\right),  \tag{27}\\
& i=2,3, \ldots, n, j=1,2,3, \ldots, n ; \nu \geq 0 .
\end{align*}
$$

Here, $X_{1}, \sum_{i}, i=2, \ldots n$ specify the integration range away from the nucleus over which the integrals of Eqs. (26) and (27) are calculated using Simpson's expansions.

Taylor expansions of $U_{s t}^{(1)}\left(x_{1}\right), \tilde{f}_{\ell}\left(k_{1} x_{1}\right)$ and $\tilde{g}_{\ell}\left(k_{1} x_{1}\right)$ are used to obtain the starting value of $f_{\ell}^{(1, j, 0)}\left(x_{1}\right)$ (see ref. [11]).

Equations (26) and (27) can be abbreviated to the following:

$$
\begin{gather*}
f_{\ell}^{(1, j, \nu)}\left(x_{1}\right)=a_{1}^{(j, \nu)} \tilde{f}_{\ell}\left(k_{1} x_{1}\right)+b_{1}^{(j, \nu)} \tilde{g}_{\ell}\left(k_{1} x_{1}\right), j=1,2,3, \ldots n ; \nu>0  \tag{28}\\
g_{\ell}^{(i, j, \nu)}\left(\sigma_{i}\right)=a_{i}^{(j, \nu)} \tilde{f}_{\ell}\left(k_{i} \sigma_{i}\right)+b_{i}^{(j, \nu)} \tilde{g}_{\ell}\left(k_{i} \sigma_{i}\right), i=2, \ldots, n, j=1,2,3, \ldots n ; \nu>0 \tag{29}
\end{gather*}
$$

The preceding coefficients of Eqs. (28) and (29) are elements of the matrices $a^{v}$ and $b^{v}$, which are given by:

$$
\left.\begin{array}{l}
\left(a^{v}\right)_{i j}=\sqrt{2 \mu_{m_{i}} / k_{i}} a_{i}^{(j, v)}  \tag{30}\\
\left(b^{v}\right)_{i j}=\sqrt{2 \mu_{m_{i}} / k_{i}} b_{i}^{(j, v)}, i, j=1,2, \ldots, n, \nu>0
\end{array}\right],
$$

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and we can obtain the reactance matrix, $R^{v}$, using the following relation:

$$
\begin{equation*}
R^{v}=b^{v}\left(a^{v}\right)^{-1}, \quad \nu>0 \tag{31}
\end{equation*}
$$

The partial cross-sections in the present work are determined (in $\pi a_{0}^{2}$ ) by:

$$
\begin{equation*}
\sigma_{i j}^{(\ell, v)}=\frac{4(2 \ell+1)}{k_{1}^{2}}\left|T_{i j}^{\nu}\right|^{2}, \quad i, j=1,2,3, \ldots, n, \quad \nu>0 \tag{32}
\end{equation*}
$$

where $k_{1}$ is the momentum of the incident protons, $\nu$ is the number of iterations, and $T_{i j}^{\nu}$ is the elements of the $n \times n$ transition matrix $T^{\nu}$, which is given by:

$$
\begin{equation*}
T^{\nu}=R^{\nu}\left(I-\tilde{i} R^{\nu}\right)^{-1}, \quad \nu>0 \tag{33}
\end{equation*}
$$

where $R^{\nu}$ is the reactance matrix and $I$ is an $n \times n$ unit matrix and $\tilde{i}=\sqrt{-1}$.
The total cross-sections (in $\pi a_{0}^{2}$ units) can be obtained (in the $\nu$ th iteration) by:

$$
\begin{equation*}
\sigma_{i j}^{\nu}=\sum_{\ell=0}^{\infty} \sigma_{i j}^{(\ell v)}, \quad i, j=1,2,3, \ldots, n, \quad \nu>0 \tag{34}
\end{equation*}
$$

## 3. Proton-lithium scattering

As an application of our MCSA, we are going to apply the above method in the case of $n=4$ (four-channels CSA) to the scattering of p-Li. Our problem can be written in the following form:

$$
p+L i(2 s)=\left[\begin{array}{ll}
p+L i(2 s) & \text { Elastic channel ( first channel) }  \tag{35}\\
H(1 s)+L i^{+} & H(1 s) \text { formation channel ( second channel) } \\
H(2 s)+L i^{+} & H(2 s) \text { formation channel ( third channel) } \\
H(2 p)+L i^{+} & H(2 p) \text { formation channel (fourth channel) }
\end{array}\right.
$$

$\Phi_{1}\left(r_{1}\right)$ is the valence electron wave function of the target (lithium) atom, which is calculated using Clementi's tables [12], and $\Phi_{i}\left(\rho_{i}\right), \quad i=2,3,4$ are the wave functions of the hydrogen formation, which are given by:

$$
\begin{equation*}
\Phi_{2}=\frac{1}{\sqrt{\pi}} \exp \left(-\rho_{2}\right), \quad \Phi_{3}=\frac{1}{\sqrt{32 \pi}}\left(2-\rho_{3}\right) \exp \left(-\rho_{3} / 2\right) \text { and } \Phi_{4}=\frac{1}{\sqrt{32 \pi}} \rho_{4} \cos \theta_{\rho_{4}, \sigma_{4}} \exp \left(-\rho_{4} / 2\right) \tag{36}
\end{equation*}
$$

## 4. Results and discussion

We start our calculations on p-Li scattering by testing the variation of the static potentials $U_{s t}^{(1)}\left(x_{1}\right)$ and $U_{s t}^{(i)}\left(\sigma_{i}\right), i=2,3,4$, of the considered channels with the increase of $x_{1}, \sigma_{i}(i=2,3,4)$. In the second step, we consider the integration range, $I R$, to be $32 a_{0}$ with Simpson's interval of 0.0625 to obtain the considered integration. It is found that excellent convergence can be obtained with Simpson's interval of $h=0.0625$, $n=512$ points, and $\nu=50$. We have calculated the total cross-sections of $\mathrm{p}-\mathrm{Li}$ scattering corresponding to $0 \leq \ell \leq 6$ at incident energies between 50 and 1000 keV . The Table shows the present total cross-sections of
Table. Present $\sigma_{12}, \sigma_{13}$, and $\sigma_{14}$ (in $\pi a_{0}^{2}$ ) of p-Li scattering with the results of [1], [2], [3], and [7].

| $\begin{aligned} & \mathrm{k}^{2} \\ & \mathrm{keV} \end{aligned}$ | Present $H(1 s)$ $\sigma_{12}$ | Banyard and Shirtcliffe <br> [1] <br> (1s) <br> (CDW) | Ferrante and <br> [2] <br> (1s) <br> (OBK) | Daniele et al. <br> [3] (1s) (eikonal) | Present H(2s) $\sigma_{13}$ | Banyard and Shirtcliffe <br> [1] <br> (2s) <br> (CDW) | Ferrante and Fiordilino [2] (2s) (OBK) | Tiwari [7] (2s) (CPB) | Present H(2p) <br> $\sigma_{14}$ | Banyard and Shirtcliffe <br> [1] <br> (2p) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 50 | $4.6753 \mathrm{E}-2$ |  |  |  | $9.0561 \mathrm{E}-3$ |  | $6.5 \mathrm{E}-1$ | $3.596 \mathrm{E}-3$ | $8.2737 \mathrm{E}-4$ |  |
| 100 | $1.9672 \mathrm{E}-2$ |  | $6.84 \mathrm{E}-3$ | $4.8947 \mathrm{E}-3$ | $4.8653 \mathrm{E}-3$ |  | $1.0 \mathrm{E}-3$ | $6.746 \mathrm{E}-4$ | $3.5363 \mathrm{E}-4$ |  |
| 150 | $1.1757 \mathrm{E}-2$ |  |  |  | $2.2135 \mathrm{E}-3$ |  | $4.9 \mathrm{E}-3$ | $1.294 \mathrm{E}-4$ | $1.5765 \mathrm{E}-4$ |  |
| 200 | $7.5246 \mathrm{E}-3$ | $8.166 \mathrm{E}-3$ | $1.873 \mathrm{E}-3$ | $5.6149 \mathrm{E}-4$ | 8.9237E-4 | $1.048 \mathrm{E}-3$ | $2.8 \mathrm{E}-3$ | $3.294 \mathrm{E}-5$ | $1.2033 \mathrm{E}-4$ | $1.467 \mathrm{E}-04$ |
| 250 | $5.4237 \mathrm{E}-3$ |  |  |  | $6.0929 \mathrm{E}-4$ |  |  | $1.327 \mathrm{E}-5$ | $9.0672 \mathrm{E}-5$ |  |
| 300 | $3.5916 \mathrm{E}-3$ |  |  |  | $3.5432 \mathrm{E}-4$ |  |  | $8.489 \mathrm{E}-6$ | $6.5326 \mathrm{E}-5$ |  |
| 350 | $2.3321 \mathrm{E}-3$ |  |  |  | $2.3564 \mathrm{E}-4$ |  |  |  | $4.6673 \mathrm{E}-5$ |  |
| 400 | $1.3622 \mathrm{E}-3$ |  |  |  | $1.5465 \mathrm{E}-4$ |  |  |  | $2.3917 \mathrm{E}-5$ |  |
| 450 | $5.7923 \mathrm{E}-4$ |  |  |  | $8.6726 \mathrm{E}-5$ |  |  |  | $8.7861 \mathrm{E}-6$ |  |
| 500 | $3.5588 \mathrm{E}-4$ | $3.878 \mathrm{E}-4$ |  |  | $4.5163 \mathrm{E}-5$ | $5.212 \mathrm{E}-5$ |  | $9.828 \mathrm{E}-7$ | $4.7005 \mathrm{E}-6$ | $5.751 \mathrm{E}-06$ |
| 550 | $2.6345 \mathrm{E}-4$ |  |  |  | $4.0872 \mathrm{E}-5$ |  |  |  | $3.2793 \mathrm{E}-6$ |  |
| 600 | $2.0526 \mathrm{E}-4$ |  |  |  | $3.2844 \mathrm{E}-5$ |  |  |  | $2.2395 \mathrm{E}-6$ |  |
| 650 | $1.6767 \mathrm{E}-4$ |  |  |  | $2.3643 \mathrm{E}-5$ |  |  |  | $1.5457 \mathrm{E}-6$ |  |
| 700 | $1.2358 \mathrm{E}-4$ |  |  |  | $1.5971 \mathrm{E}-5$ |  |  |  | $1.0823 \mathrm{E}-6$ |  |
| 750 | 8.6739E-5 |  |  |  | $9.8174 \mathrm{E}-6$ |  |  |  | $8.8835 \mathrm{E}-7$ |  |
| 800 | $5.3231 \mathrm{E}-5$ | $5.778 \mathrm{E}-5$ |  |  | $6.8517 \mathrm{E}-6$ | $7.711 \mathrm{E}-6$ |  | $2.278 \mathrm{E}-7$ | $6.5791 \mathrm{E}-7$ | $7.604 \mathrm{E}-07$ |
| 850 | $4.0683 \mathrm{E}-5$ |  |  |  | $5.3567 \mathrm{E}-6$ |  |  |  | $5.6372 \mathrm{E}-7$ |  |
| 900 | $3.0095 \mathrm{E}-5$ |  |  |  | $4.3973 \mathrm{E}-6$ |  |  |  | $4.5517 \mathrm{E}-7$ |  |
| 950 | $2.5657 \mathrm{E}-5$ |  |  |  | $3.0035 \mathrm{E}-6$ |  |  |  | $3.3423 \mathrm{E}-7$ |  |
| 1000 | $2.0139 \mathrm{E}-5$ | $2.189 \mathrm{E}-5$ |  |  | $2.4529 \mathrm{E}-6$ | $2.906 \mathrm{E}-6$ |  | $9.366 \mathrm{E}-8$ | $2.7116 \mathrm{E}-7$ | $2.716 \mathrm{E}-07$ |

p-Li scattering with those of Banyard and Shirtcliffe [1], Ferrante and Fiordilino [2], Daniele et al. [3], and Tiwari [7] in the energy range of $50-1000 \mathrm{keV}$. Our results and the available compared results in the range of energy of $500-1000 \mathrm{keV}$ are also displayed in Figures 2-4. In Figure 5 we also show the present results of the total cross-sections of the four channels (elastic and the hydrogen formation $(H$ (1s), $H$ ( $2 s$ ), $H$ (2p)) in the same range of energy $(50-1000 \mathrm{keV})$. The present values of the total cross-sections of the four channels have trends similar to the comparison results. Our values of the total cross-sections of the four channels decrease with the incident energies. The calculated total cross-sections $\sigma_{12}$ of $H(1 s)$ are about $7.85 \%-8 \%$ lower than the results of Banyard and Shirtcliffe [1]. The total cross-sections $\sigma_{13}$ of $H$ (2s) are about $11.1 \%-15.6 \%$ lower than those of Banyard and Shirtcliffe [1]. Our results of the total cross-sections $\sigma_{14}$ of $H(2 p)$ are about $13.5 \%-18.3 \%$ lower than the available values of Banyard and Shirtcliffe [1]. We also noticed that the available compared results of Ferrante and Fiordilino [2], Daniele et al. [3], and Tiwari [7] are higher than our results. The present calculations show that we have more H-formation if we open more excited channels of hydrogen formation in the collision of protons with lithium atoms. The present calculated total cross-sections have the same trend as


Figure 2. $\sigma_{12}\left(\operatorname{in} \pi a_{0}^{2}\right)$ of $\mathrm{p}-\mathrm{Li}$ scattering with those of Banyard and Shirtcliffe [1].


Figure 4. $\sigma_{14}$ ( in $\pi a_{0}^{2}$ ) of p -Li scattering with those of Banyard and Shirtcliffe [1].


Figure 3. $\sigma_{13}$ ( in $\pi a_{0}^{2}$ ) of $\mathrm{p}-\mathrm{Li}$ scattering with those of Banyard and Shirtcliffe [1].


Figure 5. $H(1 s), H(2 s)$, and $H(2 p)$ cross-sections (in $\pi a_{0}^{2}$ ) of $\mathrm{p}-\mathrm{Li}$ scattering.
the comparison results and give good agreement with the available previous results of Banyard and Shirtcliffe [1].

## 5. Conclusions

p-Li scattering was studied using MCSA as a four-channel problem (elastic, $H(1 s), H(2 s)$, and $H(2 p))$. Our interest was focused on the formation of ground, $H(1 s)$, and excited hydrogen, $H(2 s)$, and $H(2 p)$ in p-Li scattering. The difference between the four-channel problem and the three- or two-channel problems is in improving the total cross-sections of the considered channel by adding the effect of more kernels of the other three channels (in the two-channel problem, we have only one kernel, and in three channels, we have two kernels), which give more H -formation in the considered states. We expect that we can obtain more hydrogen formation if we open more channels in our calculation, which we will consider in future work.

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