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 H (1s) and excited H (in 2s- and 2p- 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 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 p-Li atoms at intermediate energies of the projectile. A numerical procedure is generalized to solve the obtained multihypercoupled equations. Throughout this paper Rydberg units are used and the total cross-sections are expressed in units of $\pi a_0^2 (= 8.8 \times 10^{-17} \text{cm}^2)$ and energy units of keV.

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

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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, $\bar{p}_i$ 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.

\[
p + A = \begin{cases} \frac{p + A}{H(n\ell) + A} & \text{Elastic channel (first channel)} \\ H(n\ell) + A & \text{formation channels ((n-1) - channels)} \end{cases},
\]

(1)

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:

\[
H = H^{(1)} = H_T - \frac{1}{2\mu_1} \nabla_{x_1}^2 + V^{(1)}_{\text{int}}(x_1) = -\frac{1}{2\mu_T} \nabla_{r_1}^2 - \frac{2}{r_1} + V_c(r_1) - \frac{1}{2\mu_1} \nabla_{x_1}^2 + V^{(1)}_{\text{int}}(x_1),
\]

(2)

where $H_T$ is the Hamiltonian of the target atom. $\mu_T$ is the reduced mass of the target atom.

\[
H = H^{(i)} = H_i - \frac{1}{2\mu_i} \nabla_{\sigma_i}^2 + V^{(i)}_{\text{int}}(\sigma_i) = -\frac{1}{2\mu_i} \nabla_{\rho_i}^2 - \frac{2}{\rho_i} + \frac{1}{2\mu_i} \nabla_{\sigma_i}^2 + V^{(i)}_{\text{int}}(\sigma_i), \quad i = 2, 3, 4, ... n
\]

(3)

The Hamiltonian of the (n-1)-rearrangement channels are expressed by:

Here, $H_i$, $i = 2, 3, 4, ... n$ are the Hamiltonians of the hydrogen formation atoms, $H(n\ell)$, respectively. $\mu_i$, $i = 2, 3, 4, ... n$ are the reduced masses of (n-1)- channels, respectively.

$V_c(r_1)$ is a screened potential and $V^{(1)}_{\text{int}}(x_1)$ is the interaction potential of the first channel, given by:

\[
V_c(r_1) = V_{c\text{Coul}}(r_1) + V_{c\text{ex}}(r_1),
\]

(4)

where $V_{c\text{Coul}}(r_1)$ and $V_{c\text{ex}}(r_1)$ are the Coulomb and exchange parts of the core potential, respectively (see ref. [11]), and

\[
V^{(1)}_{\text{int}}(x_1) = \frac{2}{x_1} - \frac{2}{\rho_1} + V_{c\text{Coul}}(x_1) \quad \text{where} \quad V_{c\text{Coul}}(x_1) = -V_{c\text{Coul}}(r_1), \quad i = 2, 3, 4, ...
\]

(5)

and $V^{(i)}_{\text{int}}(\sigma_i)$, is the interaction between the two particles of the considered hydrogen formation and the rest of the target, which is given by:

\[
V^{(i)}_{\text{int}}(\sigma_i) = \frac{2}{x_i} - \frac{2}{r_i} + V_{c\text{Coul}}(x_i) + V_{c\text{Coul}}(r_i) + V_{c\text{ex}}(r_i), \quad i = 2, 3, 4, ...
\]

(6)
The total energies \( E \) of the \( n \)-channels are defined by:

\[
E = E_i + \frac{1}{2\mu_i} k_i^2, \quad i = 1, 2, 3...n,
\]

where \( \frac{1}{2\mu_i} k_i^2 \) is the kinetic energy of the incident proton relative to the target and \( \frac{1}{2\mu_i} k_i^2, \quad i = 2, 3, 4,..., n \) 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 \( E_i, \quad i = 2, 3, 4,..., n \) refer to the binding energies of the hydrogen formation atoms, respectively.

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

\[
\langle \Phi_i | (H - E) |\Psi \rangle = 0, \quad i = 1, 2, 3,..., n.
\]

The total wave function \(|\Psi \rangle \) is expressed by

\[
|\Psi \rangle = \sum_{i=1}^{n} |\phi_i \psi_i \rangle,
\]

\[
\psi_1 = \sum_{\ell} \ell(\ell + 1)f_\ell^{(1)}(x_1)Y_{\ell}^{0}(\hat{x}_1),
\]

\[
\psi_i = \sum_{\ell} \ell(\ell + 1)g_\ell^{(i)}(\sigma_i)Y_{\ell}^{a}(\hat{\sigma}_i), \quad i = 2, 3,...n,
\]

where \( f_\ell^{(1)}(x_1) \) and \( g_\ell^{(i)}(\sigma_i), \quad i = 2, 3,...n \) are the radial wave functions of the elastic and the hydrogen formation atoms, respectively, corresponding to the total angular momentum \( \ell \). \( Y_{\ell}^{0}(x_1) \) and \( Y_{\ell}^{a}(\sigma_i) \) \( i = 2, 3,..., n \) are the related spherical harmonics. \( \hat{x}_1 \) and \( \hat{\sigma}_i \), \( i = 1, 2, 3,..., n \) are the solid angles between the vectors \( \hat{x}_1, \hat{\sigma}_i \), \( i = 2, 3,...n \) and the \( z \)-axis, respectively. \( \psi_i, \quad i = 1, 2, 3,...n \) are the corresponding scattering wave functions of the \( n \)-channels, respectively. \( \Phi_i \) is the wave function for the valence electron of the target atom, which is calculated using ref. \([12]\). \( \Phi_i, \quad i = 2, 3, 4,..., n \) 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

\[
\frac{d^2}{dx_1^2} - \frac{\ell(\ell + 1)}{x_1^2} + k_1^2 f_\ell^{(1)}(x_1) = 2\mu_1 U_{st}^{(1)}(x_1)f_\ell^{(1)}(x_1) + \sum_{\alpha=2}^{n} Q_{1\alpha}(x_1),
\]

\[
\frac{d^2}{d\sigma_i^2} - \frac{\ell(\ell + 1)}{\sigma_i^2} + k_i^2 g_\ell^{(i)}(\sigma_i) = 2\mu_i U_{st}^{(i)}(\sigma_i)g_\ell^{(i)}(\sigma_i) + \sum_{\alpha=1}^{n} Q_{i\alpha}(\sigma_i), \quad i = 2, 3,..., n,
\]

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

\[
Q_{1\alpha}(x_1) = \int K_{1\alpha}(x_1, \sigma_\alpha)g_\ell^{(\alpha)}(\sigma_\alpha)d\sigma_\alpha, \quad \alpha = 2, 3,..., n,
\]
\[
Q_{ii}(\sigma_i) = \int_0^\infty K_{i1}(\sigma_i, x_1)f^{(1)}_i(x_1)dx_1, \quad i = 2, 3, ..., n, \quad (15)
\]
\[
Q_{i\alpha}(\sigma_i) = \int_0^\infty K_{i\alpha}(\sigma_i, \sigma_\alpha)g^{(\alpha)}_i(\sigma_\alpha)d\sigma_\alpha, \quad i, \alpha = 2, 3, ..., n, \quad i \neq \alpha. \quad (16)
\]

The static potentials \(U^{(i)}_{st}(x_1)\) and \(U^{(i)}_{st}(\sigma_i)\), \(i = 2, 3, ..., n\) are defined by
\[
U^{(i)}_{st}(x_1) = \langle \Phi_1(r_1)|V^{(i)}_{int}|\Phi_1(r_1) \rangle, \quad U^{(i)}_{st}(\sigma_i) = \langle \Phi_1(\rho_i)|V^{(i)}_{int}|\Phi_1(\rho_i) \rangle. \quad (20)
\]

Eqs. (12) and (13) are inhomogeneous equations in \(x_1\), and \(\sigma_i, \ i = 1, 2, 3, ..., n\, \text{and possess the general form}
\[
(\varepsilon - H_0)\chi = \eta \quad (21)
\]

where \(\varepsilon = k_i^2(i = 1, 2, ..., n)\). \(H_0 = -\frac{\partial^2}{\partial x_i^2} + \frac{\ell(i+1)}{\sigma_i^2}\) or \(-\frac{\partial^2}{\partial x_i^2} + \frac{\ell(i+1)}{\sigma_i^2}\), \(i = 2, 3, ..., n\). \(\chi\) is \(f^{(i)}_{\ell}(x_1)\) or \(g^{(i)}_{\ell}(\sigma_i)\). \(\eta\) 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
\[
|\chi \rangle = |\chi_0 \rangle + G_0|\eta \rangle, \quad (22)
\]

where \(G_0\) is the Green operator \((\varepsilon - H_0)^{-1}\) and \(|\chi_0 \rangle\) is the solution of the homogeneous equation
\[
(\varepsilon - H_0)|\chi_0 \rangle = |0 \rangle. \quad (23)
\]

Using Green operator \(G_0\), the solutions of Eqs. (12) and (13) are given formally by
\[
f^{(1,j)}_{\ell}(x_1) = \{\delta_{j1} + \frac{1}{k_1} \int_0^\infty \tilde{g}_{\ell}(k_1x_1)[2\mu_1 U^{(1)}_{st}(x_1)f^{(1,j)}_{\ell}(x_1) + \sum_{\alpha=2}^n Q^{(j)}_{1\alpha}(x_1)]dx_1\} \tilde{f}_{\ell}(k_1x_1)

+ \{-\frac{1}{k_1} \int_0^\infty \tilde{f}_{\ell}(k_1x_1)[2\mu_1 U^{(1)}_{st}(x_1)f^{(1,j)}_{\ell}(x_1) + \sum_{\alpha=2}^n Q^{(j)}_{1\alpha}(x_1)]dx_1\} \tilde{g}_{\ell}(k_1x_1), \quad j = 1, 2, 3, ..., n \quad (24)
\]
\[ g_{\ell}^{(i,j)}(\sigma_i) = \delta_{ji} + \frac{1}{k_i} \int_{0}^{\infty} \tilde{g}_{\ell}(k_1 \sigma_i) [2\mu_i U_{st}^{(i)}(\sigma_i) g_{\ell}^{(i,j)}(\sigma_i) + \sum_{\alpha=1}^{n} Q_{i\alpha}(\sigma_i) d\sigma_i] \tilde{f}_{\ell}(k_1 \sigma_i) + \sum_{\alpha=1}^{n} Q_{i\alpha}(\sigma_i) d\sigma_i] \tilde{f}_{\ell}(k_1 \sigma_i) \]

\[ + \left\{ \frac{-1}{k_i} \int_{0}^{\infty} \tilde{f}_{\ell}(k_1 \sigma_i) [2\mu_i U_{st}^{(i)}(\sigma_i) g_{\ell}^{(i,j)}(\sigma_i) + \sum_{\alpha=1}^{n} Q_{i\alpha}(\sigma_i) d\sigma_i] \tilde{g}_{\ell}(k_1 \sigma_i), \right. \]

\[ i = 2, 3, ..., n \quad j = 1, 2, 3, ..., n \]

where \( \delta_{ji}, i, j = 1, 2, 3, ..., n \) specify two independent solutions for each of \( f_{\ell}^{(1,j)}(x_1) \) and \( g_{\ell}^{(i,j)}(\sigma_i), i = 2, 3, ..., n, \)

according to the considered channel. The functions \( \tilde{f}_{\ell}(\eta) \) and \( \tilde{g}_{\ell}(\eta), \eta = k_1 x_1, \) or \( \eta = k_1 \sigma_i \) \( i = 2, 3, ..., n \) are related to the Bessel functions of the first and second kinds, i.e. \( j_1(\eta) \) and \( y_1(\eta) \), respectively, by the relations \( \tilde{f}_{\ell}(\eta) = \eta j_1(\eta) \) and \( \tilde{g}_{\ell}(\eta) = -\eta y_1(\eta) \).

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

\[ f_{\ell}^{(1,j,\nu)}(x_1) = \delta_{ji} + \frac{1}{k_i} \int_{X_1}^{X_2} \tilde{g}_{\ell}(k_1 x_1) [2\mu_i U_{st}^{(1)}(x_1) f_{\ell}^{(1,j,\nu-1)}(x_1) + \sum_{\alpha=2}^{n} Q_{i\alpha}(\nu-1)(x_1) d\sigma_i] \tilde{f}_{\ell}(k_1 x_1) \]

\[ + \left\{ \frac{-1}{k_i} \int_{0}^{\infty} \tilde{f}_{\ell}(k_1 x_1) [2\mu_i U_{st}^{(1)}(x_1) f_{\ell}^{(1,j,\nu-1)}(x_1) + \sum_{\alpha=2}^{n} Q_{i\alpha}(\nu-1)(x_1) d\sigma_i] \tilde{g}_{\ell}(k_1 x_1), \right. \]

\[ j = 1, 2, 3, ..., n; \nu \geq 1. \]

\[ g_{\ell}^{(i,j,\nu)}(\sigma_i) = \delta_{ji} + \frac{1}{k_i} \int_{0}^{\infty} \tilde{g}_{\ell}(k_1 \sigma_i) [2\mu_i U_{st}^{(i)}(\sigma_i) g_{\ell}^{(i,j,\nu)}(\sigma_i) + \sum_{\alpha=1}^{n} Q_{i\alpha}(\nu)(\sigma_i) d\sigma_i] \tilde{f}_{\ell}(k_1 \sigma_i) \]

\[ + \left\{ \frac{-1}{k_i} \int_{0}^{\infty} \tilde{f}_{\ell}(k_1 \sigma_i) [2\mu_i U_{st}^{(i)}(\sigma_i) g_{\ell}^{(i,j,\nu)}(\sigma_i) + \sum_{\alpha=1}^{n} Q_{i\alpha}(\nu)(\sigma_i) d\sigma_i] \tilde{g}_{\ell}(k_1 \sigma_i), \right. \]

\[ i = 2, 3, ..., n, j = 1, 2, 3, ..., n; \nu \geq 0. \]

Here, \( X_1, \sum_i, i = 2, ..., n \) 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 \( U_{st}^{(1)}(x_1), \tilde{f}_{\ell}(k_1 x_1) \) and \( \tilde{g}_{\ell}(k_1 x_1) \) are used to obtain the starting value of \( f_{\ell}^{(1,j,0)}(x_1) \) (see ref. \[11]\)).

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

\[ f_{\ell}^{(1,j,\nu)}(x_1) = a_{1}^{(j,\nu)} \tilde{f}_{\ell}(k_1 x_1) + b_{1}^{(j,\nu)} \tilde{g}_{\ell}(k_1 x_1), j = 1, 2, 3, ..., n; \nu > 0 \]

\[ g_{\ell}^{(i,j,\nu)}(\sigma_i) = a_{i}^{(j,\nu)} \tilde{f}_{\ell}(k_1 \sigma_i) + b_{i}^{(j,\nu)} \tilde{g}_{\ell}(k_1 \sigma_i), i = 2, ..., n, j = 1, 2, 3, ..., n; \nu > 0 \]

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

\[ (a^{\nu})_{ij} = \sqrt{2\mu_i/k_i} a_{i}^{(j,\nu)} \]

\[ (b^{\nu})_{ij} = \sqrt{2\mu_i/k_i} b_{i}^{(j,\nu)}, i, j = 1, 2, ..., n, \nu > 0 \]

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and we can obtain the reactance matrix, $R^\nu$, using the following relation:

$$R^\nu = b^\nu (a^\nu)^{-1}, \quad \nu > 0. \quad (31)$$

The partial cross-sections in the present work are determined (in $\pi a_0^2$) by:

$$\sigma_{ij}^{(\ell,\nu)} = \frac{4(2\ell + 1)}{k_1^2} |T_{ij}^\nu|^2, \quad i, j = 1, 2, 3, ..., n, \quad \nu > 0 \quad (32)$$

where $k_1$ is the momentum of the incident protons, $\nu$ is the number of iterations, and $T_{ij}^\nu$ is the elements of the $n \times n$ transition matrix $T^\nu$, which is given by:

$$T^\nu = R^\nu (I - iR^\nu)^{-1}, \quad \nu > 0, \quad (33)$$

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:

$$\sigma_{ij}^{(\nu)} = \sum_{\ell=0}^{\infty} \sigma_{ij}^{(\ell,\nu)}, \quad i, j = 1, 2, 3, ..., n, \quad \nu > 0 \quad (34)$$

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:

$$p + Li(2s) = \begin{cases} 
  p + Li(2s) & \text{Elastic channel (first channel)} \\
  H(1s) + Li^+ & H(1s) \text{ formation channel (second channel)} \\
  H(2s) + Li^+ & H(2s) \text{ formation channel (third channel)} \\
  H(2p) + Li^+ & H(2p) \text{ formation channel (fourth channel)} 
\end{cases} \quad (35)$$

$\Phi_1(r_1)$ is the valence electron wave function of the target (lithium) atom, which is calculated using Clementi’s tables [12], and $\Phi_i(\rho_i), \quad i = 2, 3, 4$ are the wave functions of the hydrogen formation, which are given by:

$$\Phi_2 = \frac{1}{\sqrt{\pi}} \exp(-\rho_2), \quad \Phi_3 = \frac{1}{\sqrt{32\pi}} (2 - \rho_3) \exp(-\rho_3/2) \quad \text{and} \quad \Phi_4 = \frac{1}{\sqrt{32\pi}} \rho_4 \cos \theta_{\rho_4} \sigma_4 \exp(-\rho_4/2). \quad (36)$$

4. Results and discussion

We start our calculations on p-Li scattering by testing the variation of the static potentials $U_{sl}^{(1)}(x_1)$ and $U_{sl}^{(i)}(\sigma_i), \quad i = 2, 3, 4,$ of the considered channels with the increase of $x_1, \sigma_i, \quad i = 2, 3, 4$. In the second step, we consider the integration range, $IR$, to be $32a_0$ 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 p-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
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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 keV. Our results and the available compared results in the range of energy of 500–1000 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 \((H \ (1s), \ H \ (2s), \ H \ (2p))\) in the same range of energy (50–1000 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 \(H\ (1s)\) 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 \(H(2p)\) 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](image1.png)

**Figure 2.** \(\sigma_{12}\) (in \(\pi a_0^2\)) of p-Li scattering with those of Banyard and Shirtcliffe [1].

![Figure 3](image2.png)

**Figure 3.** \(\sigma_{13}\) (in \(\pi a_0^2\)) of p-Li scattering with those of Banyard and Shirtcliffe [1].

![Figure 4](image3.png)

**Figure 4.** \(\sigma_{14}\) (in \(\pi a_0^2\)) of p-Li scattering with those of Banyard and Shirtcliffe [1].

![Figure 5](image4.png)

**Figure 5.** \(H(1s), H(2s), \) and \(H(2p)\) cross-sections (in \(\pi a_0^2\)) of p-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, \(H(1s)\), \(H(2s)\), and \(H(2p)\)). Our interest was focused on the formation of ground, \(H(1s)\), and excited hydrogen, \(H(2s)\), and \(H(2p)\) 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.

References