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Complete List of Authors:	Elkilany, S.A.; Faculty of Science for girls, Ad Dammam University, ; Faculty of Science -Kafrelsheikh University, Mathematics Al-Dhawi, A.A.; University of Dammam, Mathematics Department
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Formation of non-excited and excited hydrogen in proton-lithium inelastic scattering

S A Elkilany and A A Al-Dhawi

Department of Mathematics, Faculty of Science, University of Dammam, Kingdom of Saudi Arabia.

Abstract: The collisions of proton with lithium atom are treated for the first time as a three channels problem under the assumption that the elastic and hydrogen formation in non-excited, $H(1s)$, and excited, $H(2s)$, channels are open. The effect of polarization potentials of the target and hydrogen formation is considered. A one-valence-electron model for the target, based on the Clementi-Roetti Slater-type basis functions, as well as a modified coupled-static approximation are used for calculating the partial and total cross sections of seven partial waves ($0 \leq \ell \leq 6$, where ℓ is the total angular momentum) at incident energies between 50 and 500 keV. Our values of the total cross section are in good agreement with previous results.

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Keywords: Inelastic scattering, proton-lithium, hydrogen formation, excited hydrogen formation

1. Introduction

In a recent paper [1] (to be referred to as I), we established a compact technique for treating the collisions of proton with alkali atoms as a three channels problem on the basis of the one-valence-electron model of the targets and the modified coupled-static approximation of the scattering processes. We determined the full forms of the core and static potentials by employing wavefunctions obtained by Clementi and Roetti [2] using a Roothaan-Hartree-Fock approach. This method is a modification of the two channels problem used in the effect of polarization in proton-lithium inelastic scattering [3]. Although the solutions of the scattering problems were carried out using a rather complicated method (in comparison with the first Born and the distorted wave approximations), in which the Green operators adhering to the corresponding Lippmann-Schwinger equations were expressed using partial wave expansions and iterative numerical treatment was

employed, the compactness and efficiency of the method enable us to investigate collisions of proton with lithium atom. In this case, we have 3 electrons described by the configuration $K(2) 2s$. Thus, we have orbitals of the type: $1s^2, 2s$. The Clementi-Roetti wavefunction of each s-orbital is composed of 6 components of Slater-type basis functions (see Ref. [2]). The effect of polarization potentials of the target and hydrogen formation $H(1s)$ and $H(2s)$ is considered.

2. Theoretical Formalism

The three-channels scattering problem under investigation can be described by:

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

The coupled static approximation states that the solution of the three channels scattering problem under consideration is subjected to the following conditions [1]:

$$\left[\begin{aligned} \langle \Phi_{Li(2s)} | H - E | \Psi \rangle &= 0, \\ \langle \Phi_{H(1s)} | H - E | \Psi \rangle &= 0, \\ \langle \Phi_{H(2s)} | H - E | \Psi \rangle &= 0, \end{aligned} \right] \quad (2)$$

where $|\Psi\rangle$ is the total wave function describing each scattering process, i.e.

$$|\Psi\rangle = |\Phi_{Li(2s)}\psi_1\rangle + |\Phi_{H(1s)}\psi_2\rangle + |\Phi_{H(2s)}\psi_3\rangle, \quad (3)$$

$$\Phi_{H(1s)} = \frac{1}{\sqrt{\pi}} \exp(-\rho), \quad (4)$$

and

$$\Phi_{H(2s)} = \frac{1}{\sqrt{32\pi}} (2 - \rho') \exp(-\rho'/2) \quad (5)$$

where $\psi_1(x)$ is the wave function describing scattered protons in the first channel, $\psi_2(\sigma)$ is the scattering wave function of the second channel and $\psi_3(\sigma')$ is the scattering wave function of the third channel, $\Phi_{Li(2s)}$ is the wave function for the valence electron of the target atom which is calculated using Ref. [2], $\Phi_{H(1s)}$ is the ground state wave function of hydrogen atom, $H(1s)$ and $\Phi_{H(2s)}$ is the first excited state wave function of hydrogen atom, $H(2s)$. Our results of the total cross section are obtained under the same conditions of [1](Model I) and we improved its value by considering the effect of polarization potentials of the target and hydrogen formation in our calculations ($H(1s)$ and $H(2s)$)(Model II) (see Appendix).

The partial elastic and hydrogen formation ($H(1s)$, $H(2s)$) cross sections are determined (in πa_0^2) by [1]:

$$\sigma_{ij}^{(\ell, \nu)} = \frac{4(2\ell + 1)}{k_1^2} |T_{ij}^\nu|^2, \quad i, j = 1, 2, 3 \quad (6)$$

where k_1 is the momentum of the incident protons, ν is the number of iterations and T_{ij}^ν is the elements of the 3×3 transition matrix T^ν which is connected with the reactance matrix R^ν through the relation:

$$T^\nu = R^\nu (I - \tilde{t} R) ^{-1}, \quad (7)$$

where I is a 3×3 unit matrix and $\tilde{t} = \sqrt{-1}$.

Finally, the total cross sections (in πa_0^2 units) are expressed (in ν^{th} iteration) by:

$$\sigma_{ij}^\nu = \sum_{\ell=0}^{\infty} \sigma_{ij}^{(\ell, \nu)}, \quad i, j = 1, 2, 3, \nu > 0 \quad (8)$$

3. Results and discussion

Our calculations are obtained after 50 iterations (i.e. $\nu = 50$) and integration range $IR = 32 a_0$ (remember that IR is the range away from the target nucleus to which all radial integrals are calculated using the Simpson expansions). It has been found that these conditions are enough for obtaining excellent convergence in the elements of R^ν (see Ref. [1]).

Figure 1 contains the partial and total elastic cross section, σ_{11} of Model II, for $0 \leq \ell \leq 6$ that correspond to incident energies between 50 and 250 keV. Figure 1 demonstrates the behavior of the partial elastic cross sections at all values of the total angular momentum ℓ . It also shows the important role played by the S, P and D waves at all considered incident energies. The values of the cross sections decrease steadily with k_1^2 and the seven partial waves employed are quite satisfactory for calculating them (since the higher partial waves are very small). Figure 2 involves the partial and total hydrogen formation cross sections σ_{12} of the non-excited hydrogen, $H(1s)$ of Model II. We also show the partial and total hydrogen formation cross sections σ_{13} of excited hydrogen, $H(2s)$ of Model II in figure 3. Figures 2, 3 show similar behavior of the partial and total cross sections as it is in the previous elastic results. The most interesting results of our investigations are presented in table 1 and figures 4 and 5, where we show a comparison between our values of the total cross section of $H(1s)$ and $H(2s)$ (Model I and Model II) with those determined by different authors using different approaches. Columns 2 and 3 in table 1 show the present total hydrogen formation, $H(1s)$, cross sections σ_{12} (Model I and Model II, respectively). Column 4 gives the values of the total hydrogen formation, $H(1s)$, cross sections σ_{12} obtained by Daniele et al. [4] using the eikonal-approximation (eik), developed previously within the framework of time-independent impact parameter method for high-energy proton-alkali atom charge transfer. The next two columns contain the values of the total hydrogen formation, $H(1s)$, cross sections σ_{12} of Ferrante et al. [5] using Oppenheimer, Brinkman and Kramers (OBK) and first Born approximation (FBA) approximations, respectively (see Fig. 4). Present total excited hydrogen formation, $H(2s)$, cross sections σ_{13} (Model I and Model II, respectively) are displayed in columns 7 and 8. At the last three columns, we show the values of the total excited hydrogen formation, $H(2s)$, cross sections σ_{13} obtained by Ferrante et al. [5] using OBK approximation, Banyard et al. [6] using the continuum distorted wave approximation (CDW), and by Tiwari[7] using the Coulomb projected Born (CPB), respectively (see Fig. 5). Our calculations of the total hydrogen formation, $H(1s)$, cross sections σ_{12} (Model I) show that our values of the present total cross sections are about 14-19% lower than those of Ref. [5] (FBA) at the interval of the incident energy

70–200 keV and are about 7-13% higher than those of Ref. [5] (FBA) for model II at the same interval of energy (see Fig. 4). We can also conclude that our values of the total hydrogen formation, $H(1s)$, cross sections σ_{12} of model II have the same trend and in good agreement with those of the compared results at all considered incident energies. Our results for excited hydrogen formation, $H(2s)$, cross sections σ_{13} of Model I at the interval of the incident energy 50–200 keV are about 10-22% lower than those of Ref. [7], and are about 0.4-7% lower than those of Ref. [7] (CPB) for model II on the same interval of energy except at $k_1^2 = 150$ keV our value is about 5% higher than the compared result of Ref. [7] (CPB) (see Fig. 5). From the above discussion, it may be stated that our values of the total excited hydrogen function, $H(2s)$, cross sections σ_{13} of model II have the same trend of the compared results and in good agreement with the available results.

4. Conclusions

Proton-lithium inelastic scattering is studied for the first time as a three channels problem using the modified coupled static approximation. Our interest is focused on the formation of ground, $H(1s)$, and excited hydrogen $H(2s)$. Our results of the total hydrogen formation, $H(1s)$ and $H(2s)$ (Model I) are improved by considering the polarization potentials of the target and hydrogen formation atoms, $H(1s)$ and $H(2s)$, (Model II). The difference between the three channels problem and the two channels problem is in improving the total cross sections of the considered channel by considering the effect of the two kernels of the other two channels (in two channels problem we have only one kernel). Our problem shows that three channels coupled static approximation give good agreement with previous results especially if we take the polarization potentials of the target and hydrogen formation atoms in our calculation.

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Table 1. Present total non excited hydrogen formation, $H(1s)$ cross sections (σ_{12} in πa_0^2) and total excited hydrogen formation, $H(2s)$ cross sections (σ_{13} in πa_0^2) of $p-Li$ scattering (Model I and Model II) are compared against theoretical results ([4]- [7]).

k^2 (keV)	Present σ_{12} Model I	Present σ_{12} Model II	Ref. [4] σ_{12} (eik)	Ref. [5] σ_{12} (OBK)	Ref. [5] σ_{12} (FBA)	Present σ_{13} Model I	Present σ_{13} Model II	Ref. [5] σ_{13} (OBK)	Ref. [6] σ_{13} (CDW)	Ref. [7] σ_{13} (CPB)
50	5.8693E-02	7.6673E-02				3.0989E-03	3.4818E-03	6.5E-01		3.596E-03
60	5.5421E-02	7.2531E-02				2.2312E-03	2.4709E-03			
70	4.2036E-02	5.5215E-02	1.1975E-02	7.8162E-02	5.1665E-02	1.6064E-03	1.7903E-03			
80	1.4598E-02	1.9144E-02	8.6291E-03	2.6978E-02	1.7832E-02	1.1567E-03	1.2988E-03			
90	6.1937E-03	8.1592E-03	6.4477E-03	1.1458E-02	7.5737E-03	8.3280E-04	9.3929E-04			
100	3.7011E-03	4.8892E-03	4.8947E-03	6.8400E-03	4.5212E-03	5.9961E-04	6.7204E-04	1.0E-03		6.746E-04
110	2.9396E-03	3.9045E-03	3.7748E-03	5.4443E-03	3.5986E-03	4.3172E-04	4.8867E-04			
120	2.6691E-03	3.5310E-03	2.9358E-03	4.8988E-03	3.2381E-03	3.1084E-04	3.5165E-04			
130	2.4826E-03	3.2753E-03				2.2380E-04	2.5505E-04			
140	2.2797E-03	2.9965E-03	1.8760E-03	4.1165E-03	2.7210E-03	1.6114E-04	1.8534E-04			
150	2.0605E-03	2.7020E-03				1.1602E-04	1.3532E-04	4.9E-03		1.294E-04
160	1.8422E-03	2.4092E-03	1.2191E-03	3.2779E-03	2.1667E-03	8.3534E-05	9.6048E-05			
170	1.6397E-03	2.1258E-03				6.0145E-05	6.9608E-05			
180	1.4211E-03	1.8564E-03	8.3367E-04	2.5032E-03	1.6546E-03	4.3304E-05	5.0507E-05			
190	1.2318E-03	1.6122E-03				3.1179E-05	3.6534E-05			
200	1.0658E-03	1.4000E-03	5.6149E-04	1.8730E-03	1.2380E-03	2.5849E-05	3.0662E-05	2.8E-03	1.048E-05	3.294E-05
210	5.7259E-04	7.5089E-04				1.6163E-05	1.9014E-05			
220	1.2786E-04	5.1054E-04				1.1638E-05	1.3685E-05			
230	3.4424E-04	4.5474E-04				8.3790E-06	9.9274E-06			
240	2.7079E-04	3.5967E-04				6.0329E-06	7.2153E-06			
250	2.4867E-04	3.2898E-04				4.3437E-06	5.2692E-06			1.327E-05
300	2.3485E-04	3.0984E-04				2.9857E-06	3.2451E-06			8.489E-06
350	9.4802E-06	1.2461E-05				2.0685E-06	3.0358E-06			
400	6.4581E-06	8.4688E-06				1.4869E-06	2.1945E-06			
450	4.1927E-06	5.4832E-06				1.1150E-06	1.2234E-06			
500	1.4188E-06	1.8393E-06				8.0153E-07	9.7696E-07		5.212E-07	9.828E-07

Fig. 1 Present partial and total elastic cross sections (in πa_0^2) of $p-Li$ scattering (Model II).

Fig. 2 Present partial and total $H(1s)$ formation cross sections (in πa_0^2) of $p-Li$ scattering (Model II) .

Fig. 3 Present partial and total $H(2s)$ formation cross sections (in πa_0^2) of $p-Li$ scattering (Model II).

Fig. 4 Present total $H(1s)$ formation cross sections (σ_{12} in πa_0^2) of $p-Li$ scattering are compared against theoretical results ([4] and [5]).

Fig. 5 Present total $H(2s)$ formation cross sections (σ_{13} in πa_0^2) of $p-Li$ scattering are compared against theoretical results ([5], [6] and [7]).

Appendix

The potentials $U_{st}^{(1)}(x)$, $U_{st}^{(2)}(\sigma)$ and $U_{st}^{(3)}(\sigma')$ are defined by [1]:

$$U_{st}^{(1)}(x) = \langle \Phi_{Li(2s)}(r) | V_{int}^{(1)} | \Phi_{Li(2s)}(r) \rangle, \quad (A1)$$

$$U_{st}^{(2)}(\sigma) = \langle \Phi_{H(1s)}(\rho) | V_{int}^{(2)} | \Phi_{H(1s)}(\rho) \rangle \quad (A2)$$

and

$$U_{st}^{(3)}(\sigma') = \langle \Phi_{H(2s)}(\rho') | V_{int}^{(3)} | \Phi_{H(2s)}(\rho') \rangle \quad (A3)$$

where $V_{int}^{(1)}$, $V_{int}^{(2)}$ and $V_{int}^{(3)}$ are the interaction between the particles of the three channels, respectively.

The effect of the polarization potentials of $Li(2s)$, $H(1s)$ and $H(2s)$ atoms i.e. $V_{pol}^{Li(2s)}(x)$, $V_{pol}^{H(1s)}(\sigma)$ and $V_{pol}^{H(2s)}(\sigma')$ can be carried out by replacing $U_{st}^{(1)}(x)$, $U_{st}^{(2)}(\sigma)$ and $U_{st}^{(3)}(\sigma')$ by $U^{(1)}(x)$, $U^{(2)}(\sigma)$ and $U^{(3)}(\sigma')$, respectively, such

that

$$U^{(1)}(x) = U_{st}^{(1)}(x) + V_{pol}^{Li(2s)}(x), \quad (A4)$$

$$U^{(2)}(\sigma) = U_{st}^{(2)}(\sigma) + V_{pol}^{H(1s)}(\sigma) \quad (A5)$$

and

$$U^{(3)}(\sigma') = U_{st}^{(3)}(\sigma') + V_{pol}^{H(2s)}(\sigma') \quad (A6)$$

We choose the polarization potential of the first channel, $V_{pol}^{Li(2s)}(x)$, in Peach form [8]

$$V_{pol}^{Li(2s)}(x) = -\frac{\alpha}{x^4} \left\{ 1.0 - (1.0 + \gamma x + \frac{(\gamma x)^2}{2}) e^{-\gamma x} \right\} \quad (A7)$$

where $\alpha = 0.19$ and $\gamma = 3.91$

The polarization potentials $V_{pol}^{H(1s)}(\sigma)$ of channel 2 and $V_{pol}^{H(2s)}(\sigma')$ of channel 3 are added to $U_{st}^{(2)}(\sigma)$ and $U_{st}^{(3)}(\sigma')$,

respectively, while the coupled static picture of the system is considered. $V_{pol}^{H(1s)}(\sigma)$, which is added to include all p-states

of $n = 2$, i.e. $H(1s + 2p)$ is defined by [9].

Let

$$\Phi_{H(np)}(\rho) = \left(\frac{8}{43}\right)^{\frac{1}{2}} \rho \left(1 + \frac{\rho}{2}\right) e^{-\rho},$$

(A8)

$$V^{1s}(\sigma) = \langle \Phi_{H(1s)}(\rho) | V_{\text{int}}^{(1)} | \Phi_{H(np)}(\rho) \rangle \quad (\text{A9})$$

and

$$U^{1s}(\sigma) = \langle \Phi_{H(np)}(\rho) | V_{\text{int}}^{(1)} | \Phi_{H(np)}(\rho) \rangle \quad (\text{A10})$$

then

$$V_{pol}^{H(1s)}(\sigma) = \beta^{1s}(\sigma) V^{1s}(\sigma), \quad (\text{A11})$$

The function $\beta^{1s}(\sigma)$ is calculated as follows: let $\Delta E^{1s} = E_{H(1s)} - E_{H^*}$, (where $E_{H(1s)} = -1.0 \text{ Ryd}$ is binding energy of $H(1s)$, $E_{H^*} = -21/129 \text{ Ryd}$ is the binding energy of the polarized hydrogen, and $w^{1s} = \Delta E^{1s} / V^{1s}(\sigma)$). Also, we consider the two functions $\beta^{1s\pm}$ such that $\beta^{1s\pm}(\sigma) = \frac{1}{2} \{-w^{1s} \pm ((w^{1s})^2 + 4)^{\frac{1}{2}}\}$

The adiabatic energy of $H(1s)$ within the field of a unit positive charge is found to be

$$E_{ad}^{H(1s)} = \{E_{H(1s)} + U_{st}^{(1)} + 2(\beta^{1s\pm}) V^{1s} + [E_{H^*} + U^{1s}](\beta^{1s\pm})^2\} / [1 + (\beta^{1s\pm})^2] \quad (\text{A12})$$

The correct β for calculating $V_{pol}^{H(1s)}(\sigma)$ is that one of β^{1s+} and β^{1s-} which yields a minimum value for $E_{ad}^{H(1s)}$.

We, also, have $V_{pol}^{H(2s)}(\sigma')$ for channel 3 by replacing $1s$ by $2s$ in the previous calculation and $E_{H(2s)} = -0.25 \text{ Ryd}$ which is the first excited $2s$ -state energy of hydrogen atom.