



# Formation of ground and excited hydrogen atoms in proton–potassium inelastic scattering

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**Abstract.** The inelastic scattering of proton with a potassium atom is treated for the first time as a three-channel problem within the framework of the improved coupled static approximation by assuming that the ground ( $1s$  state) and the excited ( $2s$  state) hydrogen formation channels are open for seven values of total angular momentum,  $\ell$  ( $0 \leq \ell \leq 6$ ) at energies between 50 and 500 keV. The Lipmann–Swinger equation and the Green’s function iterative numerical method are used to calculate iterative partial and total cross-sections. This can be done by calculating the reactance matrix at different values of the considered incident energies to obtain the transition matrix that gives partial and total cross-sections. Present results are in reasonable agreement with previous results.

**Keywords.** Inelastic scattering; proton–potassium; hydrogen formation.

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## 1. Introduction

The appearance of intermediate states in atomic and nuclear reactions is considered as the most interesting physical phenomenon since the development of the quantum theory. The development of the femtosecond laser has tremendously enhanced the experimental identification of these states in chemical and physical reactions. Most theoretical treatments of electron–, positron– and proton–atom interactions are based on the calculations of differential, partial and total cross-sections as functions of incident energies using different approximations. It is well known that hydrogen formation plays an important role in the scattering of proton from alkali atoms at low and intermediate impact energies. Theoretical investigation on electron–, positron– and proton–atom scattering has been carried out by many researchers. Abdel-Raouf [1] applied the coupled-static and frozen core approximations to positron–lithium and positron–sodium scattering as a two-channel problem. El-Bakry and Abdel-Raouf [2] applied coupled static approximation to the production of positronium in positron–lithium scattering as a three-channel problem. Elkilany and Abdel-Raouf [3] investigated the effect of polarization potentials on

antiproton scattered by positronium using the coupled static model. Elkilany [4,5] treated in detail the effect of polarization potential on inelastic scattering of proton–lithium or proton–sodium as a two-channel problem, using the improved coupled-static approximation. Banyard and Shirtcliffe [6] used the continuum-distorted wave method to calculate cross-sections for protons scattered from atomic lithium. Ferrante *et al* [7] calculated total cross-sections for hydrogen formation in proton scattering with alkali atoms using the Oppenheimer–Brinkman–Kramer’s (OBK) approximation. Daniele *et al* [8] calculated total cross-sections of proton scattering by alkali atoms using eikonal approximation treatment, developed previously within the framework of the time-dependent impact parameter method for high-energy charge transfer. Ferrante and Fiordilino [9] investigated high-energy proton–alkali atom collision using Eikonal approximation. Fritsch and Lin [10] discussed the hydrogen formation in proton scattering by lithium atoms using a modified two-centre atomic orbital expansion. Choudhury and Sural [11] calculated the hydrogen formation cross-sections in the collision of protons with alkali metal atoms using the wave formulation of impulse approximation. Tiwari [12] reported the differential and total

cross-sections in the hydrogen formation in the collision of protons with lithium and sodium atoms using the Coulomb-projected Born approximation.

In this paper, we modify the coupled static approximation used in refs [1–5] to investigate the inelastic scattering of a proton by a potassium atom as a three-channel problem. The formation of ground and excited hydrogen are investigated in proton–potassium (p–K) inelastic scattering as a three-channel problem in which the elastic and hydrogen (in 1s and 2s states) formation channels are open for seven values of the total angular momentum  $\ell$  ( $0 \leq \ell \leq 6$ ) at energies between 50 and 500 keV. The target is described using Roothaan–Hartree–Fock atomic wave functions within the framework of the one-valence-electron model [13]. The iterative Green’s function partial-wave expansion technique is used. The next section contains a brief presentation of our mathematical formalism, §3 is devoted to the discussions of our results and a conclusion on the present results is given in §4. The appendices involve a short treatment of the methods that are used in calculating the reactance matrix (Appendix A) and the numerical iterative method (Appendix B), which are used in calculating the integrals of our problem.

## 2. Theoretical formalism

The three-channel scattering problem under investigation can be sketched by (see figure 1)

$$p + K(4s) = \begin{cases} p + K(4s) & \text{Elastic channel} \\ & \text{(first channel)} \\ H(1s) + K^+ & \text{H(1s) formation} \\ & \text{(second channel)} \\ H(2s) + K^+ & \text{H(2s) formation} \\ & \text{channel (third channel)} \end{cases} \quad (1)$$

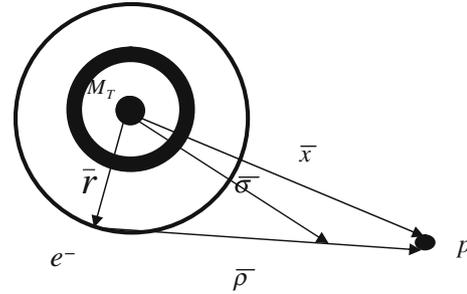
The one-valence-electron model of the target, K, is described (in Rydberg units, Ry) by the Hamiltonian [1]:

$$H_T = -\frac{1}{2\mu_m} \nabla_r^2 - \frac{2}{r} + V_c(r), \quad (2)$$

where  $r$  is the position vector of the valence electron with respect to the origin of the scattering system in which the nucleus of the target is infinitely heavy,  $\mu_m$  is the reduced mass of the target and  $V_c(r)$  is a screened potential defined by

$$V_c(r) = V_{c\text{Coul}}(r) + V_{c\text{ex}}(r), \quad (3)$$

where  $V_{c\text{Coul}}(r)$  and  $V_{c\text{ex}}(r)$  are the Coulomb and exchange parts of the core potential, respectively.



**Figure 1.** Configuration space of p–K(4s) scattering:  $\bar{x}$  and  $\bar{r}$  are the position vectors of the projectile proton and the valence electron of the target with respect to the centre of mass of the target,  $\bar{\rho}$  is the position vector of the projectile proton with respect to the valence electron of the target,  $\bar{\sigma}$  is the position vector of the centre of mass of H from the target,  $M_T$  is the mass of the nucleus of the target.

Using Clementi and Roetti Tables [13], the wave function of the  $i$ th electron in the orbital  $j$  of the target is expanded by

$$\Phi_j(r_i) = \sum_{p=1}^{m_j} c_{jp} \chi_{jp}(r_i), \quad (4)$$

where  $|\chi_{jp}(r_i)\rangle$  is a Slater-type wave function given by

$$\chi_{jp}(r_i) = A_{jp} r_i^{k_{jp}} e^{-\alpha_{jp} r_i} Y_{jp}(\vartheta_i, \varphi_i). \quad (5)$$

The  $k_{jp}$  are integers or zero and  $A_{jp}$  are normalization factors determined by

$$A_{jp} = [(2\alpha_{jp})^{2k_{jp}+1} / (2k_{jp}!)]^{1/2} \quad (6)$$

and the spherical harmonics  $Y_{jp}$  are normalized by  $\langle Y_{jp}(\vartheta_i, \varphi_i) | Y_{jp}(\vartheta_i, \varphi_i) \rangle = 1$ . The constants  $c_{jp}$  and  $\alpha_{jp}$  are adjusted within the framework of the Hartree–Fock–Roothaan approach. Substituting eq. (5) into eq. (4) and introducing the notation  $\bar{c}_{jp} = c_{jp} A_{jp}$ , we obtain

$$\Phi_j(r_i) = \sum_{p=1}^{m_j} \bar{c}_{jp} r_i^{k_{jp}} e^{-\alpha_{jp} r_i} Y_{jp}(\vartheta_i, \varphi_i), \quad (7)$$

where  $m_j$  in eqs (4) and (7) is the number of basis functions characteristic to each orbital (usually, all orbitals of the same type have the same  $m_j$ ).

The Coulomb part of the core potential is defined by

$$V_{c\text{Coul}}(r) = \sum_{j=1}^M N_j \left\langle \Phi_j(r_i) \left| \frac{2}{|\bar{r} - \bar{r}_i|} - \frac{2}{r} \right| \Phi_j(r_i) \right\rangle, \quad (8)$$

where  $M$  is the number of orbitals and  $N_j$  is the number of electrons occupying the orbital  $j$ . The prime on the summation sign means that the term  $-2/r$  is repeated

for each  $j$ . The exchange part of the core potential is defined by

$$V_{\text{cex}}(r) = - \sum_{j=1}^M \left\langle \Phi_{\text{K}(4s)}(r_i) \left| \frac{2}{|\bar{r} - \bar{r}_i|} \right| \Phi_j(r_i) \right\rangle, \quad (9)$$

where the subscript  $\text{K}(4s)$  is employed for distinguishing the wave function for the valence electron of the target atom. According to eq. (2), the binding energy of the valence electron of the target is determined by

$$E_{\text{K}(4s)} = \langle \Phi_{\text{K}(4s)}(r) | H_{\text{T}} | \Phi_{\text{K}(4s)}(r) \rangle. \quad (10)$$

The total Hamiltonian of the first channel, elastic channel (in Rydberg units and frozen core approximation) has the following form:

$$H = H^{(1)} = H_{\text{T}} - \frac{1}{2\mu_{\text{M}}} \nabla_x^2 + V_{\text{int}}^{(1)}, \quad (11)$$

where  $\mu_{\text{M}}$  is the reduced mass of the first channel and  $V_{\text{int}}^{(1)}$  denotes the interaction between the incident proton and the target atom. That is,

$$V_{\text{int}}^{(1)} = \frac{2}{x} - \frac{2}{|\bar{x} - \bar{r}|} + V_{\text{cCoul}}(x), \quad (12)$$

where

$$V_{\text{cCoul}}(x) = -V_{\text{cCoul}}(r)|_{r=x}, \quad (13)$$

and the corresponding total energy in the first channel is determined by

$$E = E^{(1)} = E_{\text{K}(4s)} + \frac{1}{2\mu_{\text{M}}} k_1^2, \quad (14)$$

where  $(1/2\mu_{\text{M}})k_1^2$  is the kinetic energy of the incident proton relative to the target nucleus.

The total Hamiltonian of the second channel,  $\text{H}(1s)$ , formation is expressed (in Rydberg units and frozen core approximation) as

$$H = H^{(2)} = H_{\text{H}(1s)} - \frac{1}{2\mu_{\text{M}'}} \nabla_{\sigma}^2 + V_{\text{int}}^{(2)}, \quad (15)$$

where  $\mu_{\text{M}'}$  is the reduced mass of the second channel and  $V_{\text{int}}^{(2)}$  represents the interaction between the particles of  $\text{H}(1s)$  and the rest of the target atom. That is,

$$V_{\text{int}}^{(2)} = \frac{2}{x} - \frac{2}{r} + V_{\text{cCoul}}(x) + V_{\text{cCoul}}(r) + V_{\text{cex}}(r), \quad (16)$$

and the total energy of the second channel is determined by

$$E = E^{(2)} = E_{\text{H}(1s)} + \frac{1}{2\mu_{\text{M}'}} k_2^2, \quad (17)$$

where  $(1/2\mu_{\text{M}'})k_2^2$  is the kinetic energy of the centre of mass of  $\text{H}(1s)$  with respect to the nucleus of the target. This is related to the energy of the incident proton by

$$\frac{k_2^2}{2\mu_{\text{M}'}} = \left( E_{\text{K}(4s)} + \frac{1}{2\mu_{\text{M}}} k_1^2 - E_{\text{H}(1s)} \right), \quad (18)$$

where  $E_{\text{H}(1s)} = -1.0$  Ry is the ground state energy of  $\text{H}(1s)$  and  $(k_2^2/2\mu_{\text{M}'}) > 0$  means that the  $\text{H}(1s)$  channel is open, otherwise it is closed. Thus,  $\text{H}(1s)$  formation is only possible if  $k_1^2 > 2\mu_{\text{M}}(E_{\text{H}(1s)} - E_{\text{K}(4s)})$ .

The total Hamiltonian of the third channel,  $\text{H}(2s)$  formation, is expressed (in Rydberg units and frozen core approximation) as

$$H = H^{(3)} = H_{\text{H}(2s)} - \frac{1}{2\mu_{\text{M}''}} \nabla_{\sigma'}^2 + V_{\text{int}}^{(3)}, \quad (19)$$

where  $\mu_{\text{M}''}$  is the reduced mass of the third channel and  $V_{\text{int}}^{(3)}$  represents the interaction between the particles of  $\text{H}(2s)$  and the rest of the target atom. That is,

$$V_{\text{int}}^{(3)} = \frac{2}{x'} - \frac{2}{r'} + V_{\text{cCoul}}(x') + V_{\text{cCoul}}(r') + V_{\text{cex}}(r'), \quad (20)$$

and the total energy of third channel is determined by

$$E = E^{(3)} = E_{\text{H}(2s)} + \frac{1}{2\mu_{\text{M}''}} k_3^2, \quad (21)$$

where  $(1/2\mu_{\text{M}''})k_3^2$  is the kinetic energy of the centre of mass of  $\text{H}(2s)$  with respect to the nucleus of the target. This is related to the energy of the incident proton by

$$\frac{k_3^2}{2\mu_{\text{M}''}} = \left( E_{\text{K}(4s)} + \frac{1}{2\mu_{\text{M}}} k_1^2 - E_{\text{H}(2s)} \right), \quad (22)$$

where  $E_{\text{H}(2s)} = -0.25$  Ry is the first excited state energy of the excited  $\text{H}(2s)$  and  $(k_3^2/2\mu_{\text{M}''}) > 0$  means that  $\text{H}(2s)$  channel is open, otherwise it is closed. Thus,  $\text{H}(2s)$  formation is only possible if  $k_1^2 > 2\mu_{\text{M}}(E_{\text{H}(2s)} - E_{\text{K}(4s)})$ .

The coupled static approximation states that the solution of the three-channel scattering problem under consideration is subjected to the following conditions:

$$\langle \Phi_{\text{K}(4s)} | H - E | \Psi \rangle = 0, \quad (23)$$

$$\langle \Phi_{\text{H}(1s)} | H - E | \Psi \rangle = 0, \quad (24)$$

$$\langle \Phi_{\text{H}(2s)} | H - E | \Psi \rangle = 0, \quad (25)$$

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

$$|\Psi\rangle = |\Phi_{\text{K}(4s)}(r)\rangle |\psi_1(x)\rangle + |\Phi_{\text{H}(1s)}(\rho)\rangle |\psi_2(\sigma)\rangle \\ \times |\Phi_{\text{H}(2s)}(\rho')\rangle |\psi_3(\sigma')\rangle, \quad (26)$$

$$\Phi_{H(1s)} = \frac{1}{\sqrt{\pi}} \exp(-\rho), \quad (27)$$

$$\Phi_{H(2s)} = \frac{1}{\sqrt{32\pi}} (2 - \rho') \exp(-\rho'/2), \quad (28)$$

where  $\Phi_{H(1s)}$  is the ground-state wave function of H(1s),  $\Phi_{H(2s)}$  is the first excited state wave function of H(2s),  $\psi_1(x)$  is the wave function describing scattered protons,  $\psi_2(\sigma)$  is the scattering wave function of the second channel and  $\psi_3(\sigma')$  is the scattering wave function of the third channel. Substituting eqs (14) and (26) in eq. (23), we obtain

$$\begin{aligned} \frac{1}{2\mu_M} (\nabla_x^2 + k_1^2) |\psi_1\rangle &= U_{st}^{(1)}(x) |\psi_1\rangle + \langle \Phi_{K(4s)} | \\ &\times H^{(2)} - E^{(2)} | \Phi_{H(1s)} \psi_2 \rangle \\ &+ \langle \Phi_{K(4s)} | H^{(3)} - E^{(3)} \\ &\times | \Phi_{H(2s)} \psi_3 \rangle. \end{aligned} \quad (29)$$

Substituting eqs (17) and (26) in eq. (24), we obtain

$$\begin{aligned} \frac{1}{2\mu_{M'}} (\nabla_\sigma^2 + k_2^2) |\psi_2\rangle &= U_{st}^{(2)}(\sigma) |\psi_2\rangle + \langle \Phi_{H(1s)} | \\ &\times H^{(1)} - E^{(1)} | \Phi_{K(4s)} \psi_1 \rangle \\ &+ \langle \Phi_{H(1s)} | H^{(3)} - E^{(3)} \\ &\times | \Phi_{H(2s)} \psi_3 \rangle. \end{aligned} \quad (30)$$

Substituting eqs (21) and (26) in eq. (25), we obtain

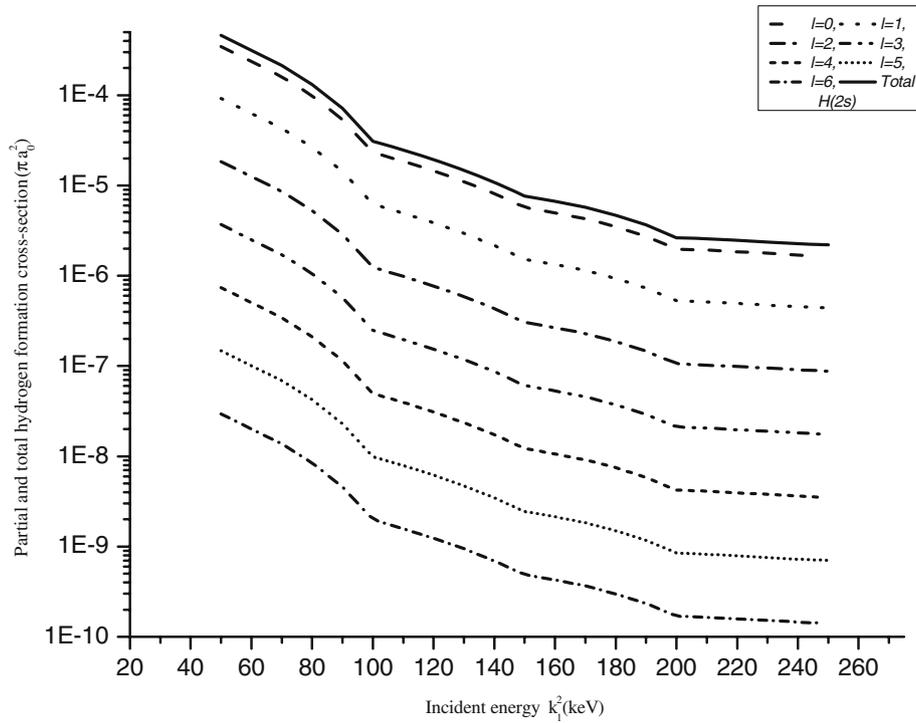
$$\begin{aligned} \frac{1}{2\mu_{M''}} (\nabla_{\sigma'}^2 + k_2^2) |\psi_3\rangle &= U_{st}^{(3)}(\sigma') |\psi_3\rangle + \langle \Phi_{H(2s)} | \\ &\times H^{(1)} - E^{(1)} | \Phi_{K(4s)} \psi_1 \rangle \\ &+ \langle \Phi_{H(2s)} | H^{(2)} - E^{(2)} \\ &\times | \Phi_{H(1s)} \psi_2 \rangle, \end{aligned} \quad (31)$$

where Schrödinger's equations of the target, H(1s) and H(2s) are employed. The potentials  $U_{st}^{(1)}(x)$ ,  $U_{st}^{(2)}(\sigma)$  and  $U_{st}^{(3)}(\sigma')$  are defined by

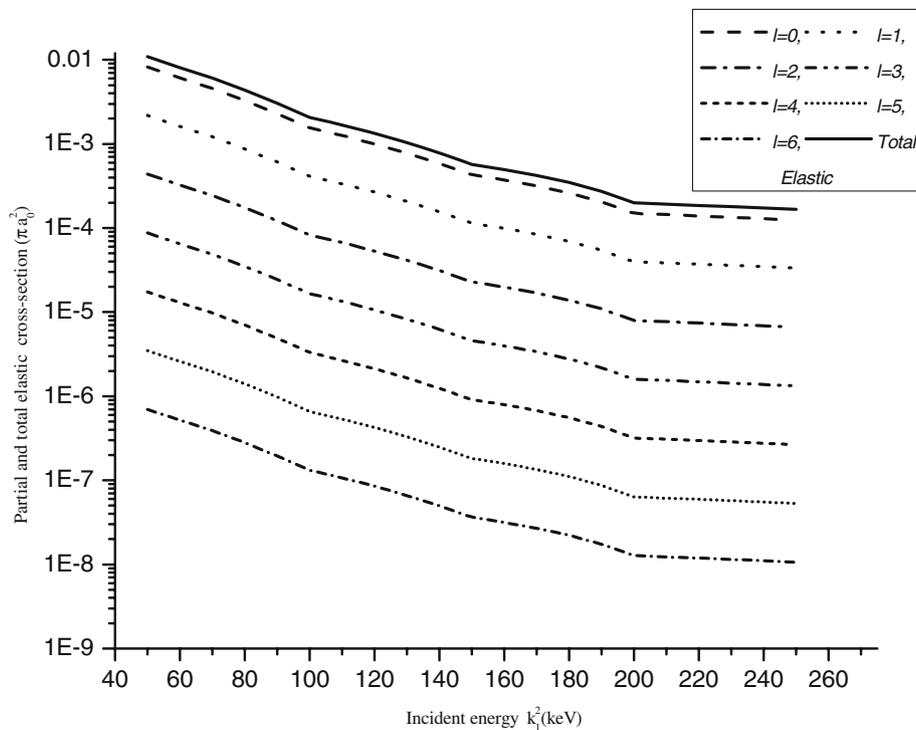
$$U_{st}^{(1)}(x) = \langle \Phi_{K(4s)}(r) | V_{\text{int}}^{(1)} | \Phi_{K(4s)}(r) \rangle, \quad (32)$$

**Table 1.** Present partial and total hydrogen formation, H(2s), cross-sections (in  $\pi a_0^2$ ) of p-K scattering.

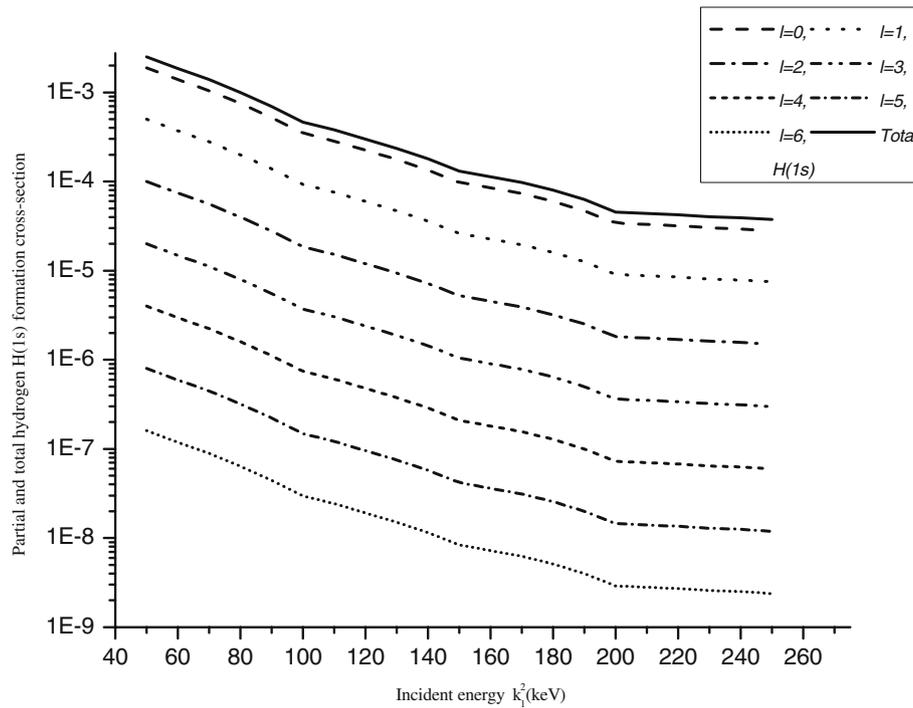
$k^2$ (keV)	$\ell = 0$	$\ell = 1$	$\ell = 2$	$\ell = 3$	$\ell = 4$	$\ell = 5$	$\ell = 6$	Total cross- section
50	3.4601E-04	9.2269E-05	1.8454E-05	3.6907E-06	7.3815E-07	1.4763E-07	2.9526E-08	4.6134E-04
60	2.3493E-04	6.2647E-05	1.2529E-05	2.5059E-06	5.0118E-07	1.0024E-07	2.0047E-08	3.1323E-04
70	1.6081E-04	4.2883E-05	8.5765E-06	1.7153E-06	3.4306E-07	6.8612E-08	1.3722E-08	2.1441E-04
80	9.9233E-05	2.6462E-05	5.2924E-06	1.0585E-06	2.1170E-07	4.2340E-08	8.4679E-09	1.3231E-04
90	5.3821E-05	1.4352E-05	2.8704E-06	5.7409E-07	1.1482E-07	2.2964E-08	4.5927E-09	7.1760E-05
100	2.3229E-05	6.1945E-06	1.2389E-06	2.4778E-07	4.9556E-08	9.9112E-09	1.9822E-09	3.0972E-05
110	1.8490E-05	4.9308E-06	9.8615E-07	1.9723E-07	3.9446E-08	7.8892E-09	1.5778E-09	2.4653E-05
120	1.4519E-05	3.8719E-06	7.7437E-07	1.5487E-07	3.0975E-08	6.1950E-09	1.2390E-09	1.9359E-05
130	1.1050E-05	2.9467E-06	5.8934E-07	1.1787E-07	2.3574E-08	4.7147E-09	9.4295E-10	1.4733E-05
140	8.1242E-06	2.1665E-06	4.3329E-07	8.6658E-08	1.7332E-08	3.4663E-09	6.9327E-10	1.0832E-05
150	5.7228E-06	1.5261E-06	3.0522E-07	6.1044E-08	1.2209E-08	2.4417E-09	4.8835E-10	7.6303E-06
160	4.9915E-06	1.3311E-06	2.6621E-07	5.3243E-08	1.0649E-08	2.1297E-09	4.2594E-10	6.6553E-06
170	4.2859E-06	1.1429E-06	2.2858E-07	4.5717E-08	9.1433E-09	1.8287E-09	3.6573E-10	5.7145E-06
180	3.4969E-06	9.3252E-07	1.8650E-07	3.7301E-08	7.4602E-09	1.4920E-09	2.9841E-10	4.6625E-06
190	2.7404E-06	7.3077E-07	1.4615E-07	2.9231E-08	5.8462E-09	1.1692E-09	2.3385E-10	3.6538E-06
200	1.9829E-06	5.2877E-07	1.0575E-07	2.1151E-08	4.2301E-09	8.4603E-10	1.6921E-10	2.6438E-06
210	1.9219E-06	5.1251E-07	1.0250E-07	2.0500E-08	4.1001E-09	8.2002E-10	1.6400E-10	2.5625E-06
220	1.8473E-06	4.9261E-07	9.8521E-08	1.9704E-08	3.9408E-09	7.8817E-10	1.5763E-10	2.4630E-06
230	1.7770E-06	4.7387E-07	9.4774E-08	1.8955E-08	3.7910E-09	7.5819E-10	1.5164E-10	2.3693E-06
240	1.7018E-06	4.5381E-07	9.0762E-08	1.8152E-08	3.6305E-09	7.2609E-10	1.4522E-10	2.2690E-06
250	1.6457E-06	4.3886E-07	8.7771E-08	1.7554E-08	3.5108E-09	7.0217E-10	1.4043E-10	2.1942E-06
300	1.3295E-06	3.5453E-07	7.0905E-08	1.4181E-08	2.8362E-09	5.6724E-10	1.1345E-10	1.7726E-06
350	1.0123E-06	2.6995E-07	5.3991E-08	1.0798E-08	2.1596E-09	4.3192E-10	8.6385E-11	1.3497E-06
400	6.9124E-07	1.8433E-07	3.6866E-08	7.3732E-09	1.4746E-09	2.9493E-10	5.8986E-11	9.2164E-07
450	3.6852E-07	9.8273E-08	1.9655E-08	3.9309E-09	7.8619E-10	1.5724E-10	3.1447E-11	4.9136E-07
500	4.4052E-08	1.1747E-08	2.3495E-09	4.6989E-10	9.3978E-11	1.8796E-11	3.7591E-12	5.8735E-08



**Figure 2.** Present partial and total hydrogen formation,  $H(2s)$ , cross-sections (in  $\pi a_0^2$ ) of p–K scattering.



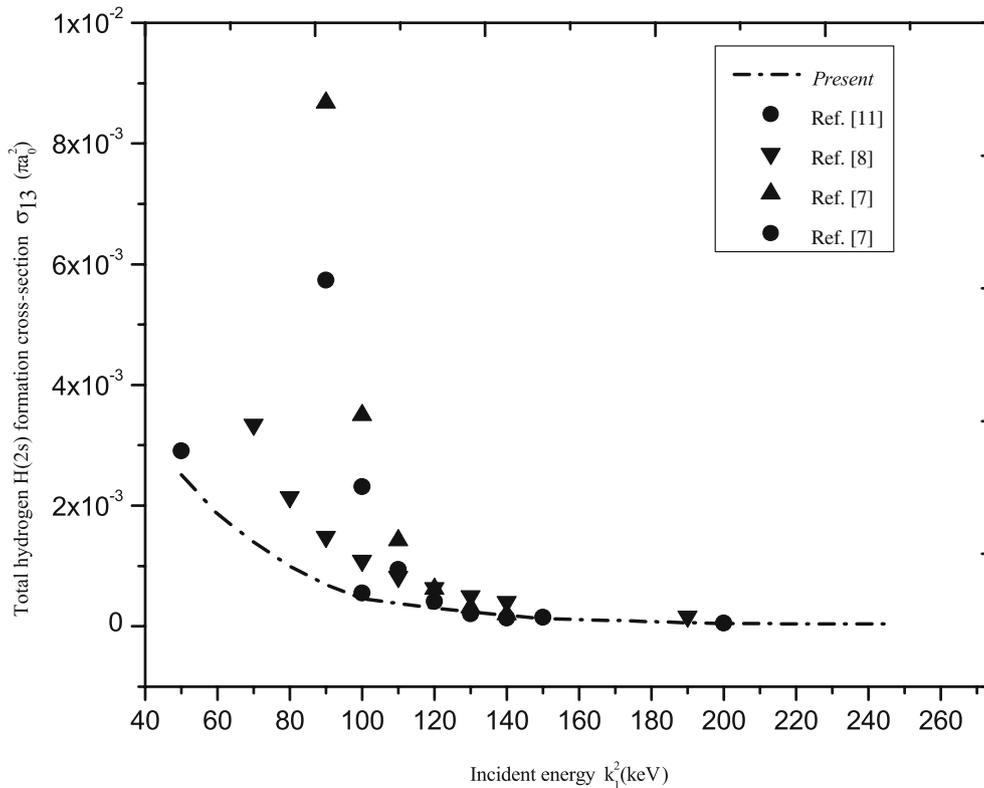
**Figure 3.** Present partial and total elastic cross-sections (in  $\pi a_0^2$ ) of p–K scattering.



**Figure 4.** Present partial and total hydrogen formation,  $H(1s)$ , cross-sections (in  $\pi a_0^2$ ) of p–K scattering.

**Table 2.** Present total cross-sections (in  $\pi a_0^2$ ) of p–K scattering with the compared results [7,8,11].

$k^2$ (keV)	$\sigma_{12}$ $H(1s)$	[7] OBK	[7] FBA	[8] Eikonal	[11]	$\sigma_{13}$ $H(2s)$	[11]
50	2.5110E-03				2.91E-03	4.6134E-04	6.38E-04
60	1.8570E-03					3.1323E-04	
70	1.3921E-03	6.4472E-02	4.2616E-02	3.3418E-03		2.1441E-04	
80	9.9991E-04	2.3499E-02	1.5532E-02	2.1390E-03		1.3231E-04	
90	6.9463E-04	8.6771E-03	5.7355E-03	1.4809E-03		7.1760E-05	
100	4.6494E-04	3.4992E-03	2.3130E-03	1.0862E-03	5.51E-04	3.0972E-05	4.34E-05
110	3.7955E-04	1.4238E-03	9.4113E-04	8.1830E-04		2.4653E-05	
120	2.9975E-04	6.2224E-04	4.1130E-04	6.3421E-04		1.9359E-05	
130	2.3552E-04	3.1496E-04	2.0819E-04	5.0283E-04		1.4733E-05	
140	1.7939E-04	1.9961E-04	1.3950E-04	4.0536E-04		1.0832E-05	
150	1.3045E-04				1.52E-04	7.6303E-06	1.06E-05
160	1.1309E-04					6.6553E-06	
170	9.7598E-05					5.7145E-06	
180	7.9902E-05					4.6625E-06	
190	6.2661E-05			1.5908E-04		3.6538E-06	
200	4.5405E-05				5.30E-05	2.6438E-06	3.68E-06
210	4.3946E-05					2.5625E-06	
220	4.2325E-05					2.4630E-06	
230	4.0330E-05					2.3693E-06	
240	3.9093E-05					2.2690E-06	
250	3.7385E-05					2.1942E-06	
300	3.0467E-05					1.7726E-06	
350	2.3289E-05					1.3497E-06	
400	1.5708E-05					9.2164E-07	
450	8.2370E-06					4.9136E-07	
500	8.2923E-07				9.55E-07	5.8735E-08	8.05E-08



**Figure 5.** Present total hydrogen, H(1s), formation cross-sections ( $\sigma_{12}$  in  $\pi a_0^2$ ) of p-K scattering in comparison with theoretical results [7,8,11].

$$U_{st}^{(2)}(\sigma) = \langle \Phi_{H(1s)}(\rho) | V_{int}^{(2)} | \Phi_{H(1s)}(\rho) \rangle \quad (33)$$

and

$$U_{st}^{(3)}(\sigma') = \langle \Phi_{H(2s)}(\rho') | V_{int}^{(3)} | \Phi_{H(2s)}(\rho') \rangle. \quad (34)$$

Using partial wave expansions of the scattering wave functions  $|\psi_1\rangle$ ,  $|\psi_2\rangle$  and  $|\psi_3\rangle$  in eqs (23)–(25), solutions are given (formally) by Lippmann–Schwinger equation (see Appendix A):

$$|\xi\rangle = |\xi_0\rangle + G_0 |\zeta\rangle, \quad (35)$$

where  $G_0$  is the Green operator  $(\varepsilon - H_0)^{-1}$  and  $|\xi_0\rangle$  is the solution of the homogeneous equation:

$$(\varepsilon - H_0) |\xi_0\rangle = |0\rangle. \quad (36)$$

The partial wave expansions of the Green operators corresponding to operators in the three differential equations enable us to write their solutions in integral form, which can be solved using the iterative numerical technique. Then we obtain reactance matrix  $R^\nu$  that is related to transition matrix  $T^\nu$  by

$$T^\nu = R^\nu (I - \tilde{i}R)^{-1}, \quad (37)$$

where  $\nu$  is the order of iteration,  $I$  is a  $3 \times 3$  unit matrix and  $\tilde{i} = \sqrt{-1}$ . Partial cross-sections obtained in an iterative way are determined (in  $\pi a_0^2$  units) by

$$\sigma_{ij}^{(\ell,\nu)} = \frac{4(2\ell + 1)}{k_1^2} |T_{ij}^\nu|^2, \quad i, j = 1, 2, 3. \quad (38)$$

Finally, the total cross-sections (in  $\pi a_0^2$  units) are expressed (in  $\nu$ th iteration) by

$$\sigma_{ij}^\nu = \sum_{\ell=0}^{\infty} \sigma_{ij}^{(\ell,\nu)}, \quad i, j = 1, 2, 3, \nu > 0. \quad (39)$$

### 3. Results and discussion

We begin by testing the variation of static potentials of three channels,  $U_{st}^{(1)}(x)$ ,  $U_{st}^{(2)}(\sigma)$  and  $U_{st}^{(3)}(\sigma')$ , with increasing  $x$ ,  $\sigma$  and  $\sigma'$ , respectively. Values of  $x$ ,  $\sigma$  and  $\sigma'$  have been chosen such that

$$x = \sigma = \sigma' = \frac{1}{16}, \frac{2}{16}, \frac{3}{16}, \dots, \frac{512}{16}$$

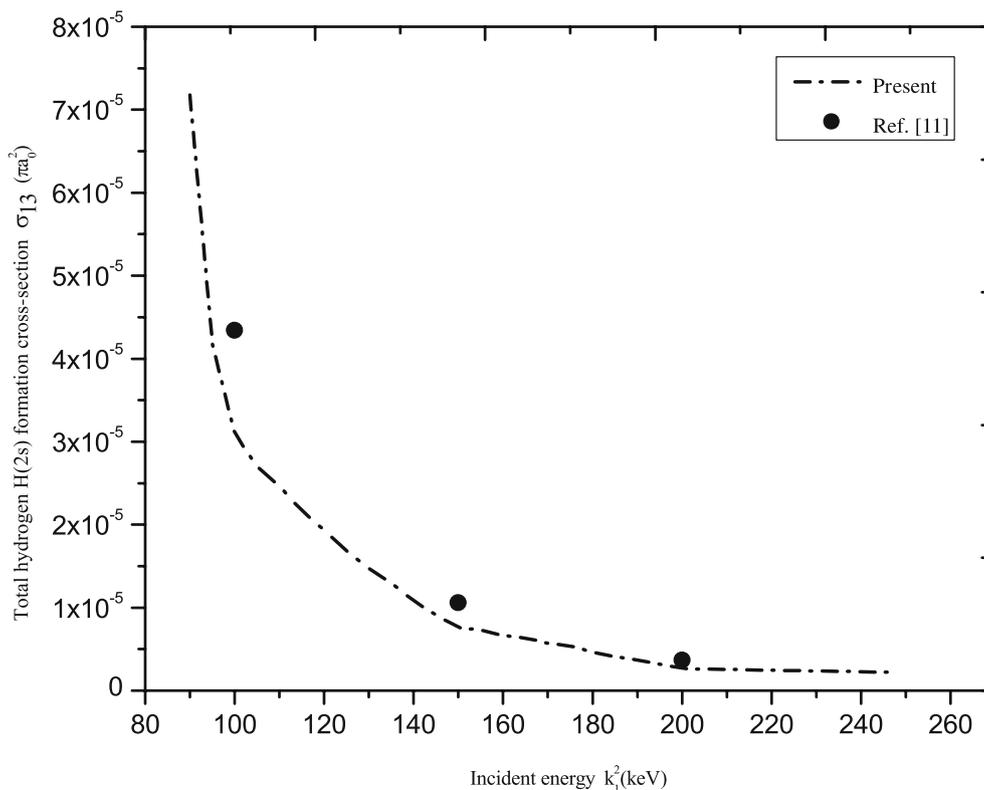
where  $h = 1/16$  is the mesh size (or Simpson’s step) employed to calculate integrals appearing in integral

equations using Simpson's rule. Calculation of cross-sections of p–K scattering has been proceeded by investigating variation of the elements of  $R^\nu$  with the increase of integration range (IR) and the number of iterations. We set  $h$  to be  $1/16$  and use 512 mesh (that is,  $IR = 32a_0$ , see Appendix B). It is found that 50 iterations are enough for the convergence of the reactance matrix elements and the partial cross-sections values; this demonstrates stability of our iterative method. Final calculations were carried out for seven partial waves corresponding to  $0 \leq \ell \leq 6$ , which are quite satisfactory for calculating the total elastic and hydrogen formation, H(1s) and H(2s) cross-sections (because the main contributions of those values are due to S, P and D partial cross-sections and at higher  $\ell$  we have very small values of the partial cross-sections) at values of  $k_1^2$ , representing the kinetic energy region ( $50 \leq k_1^2 \leq 500$  keV).

In table 1, we present the partial and total H(2s) formation cross-sections,  $\sigma_{13}$  (channel 3) at all incident values of energy between 50 and 500 keV. These values are also displayed in figure 2. We can conclude the following points:

- (1) The main contributions to the total H(2s) formation cross-sections,  $\sigma_{13}$ , are due to the S, P and D partial cross-sections.
- (2) The partial cross-sections of H(2s) formation decrease steadily with the angular momentum  $\ell$ .
- (3) The total H(2s) formation cross-sections,  $\sigma_{13}$ , decrease steadily with  $k_1^2$ .
- (4) The seven partial waves employed are quite satisfactory for calculating the total H(2s) formation cross-sections,  $\sigma_{13}$ , to a higher degree of accuracy within the framework of the improved coupled static approximation.

The common features of the obtained values of the partial and total hydrogen formation, H(2s) (channel 3), are repeated for the partial and total elastic cross-sections (channel 1) and the partial and total H(2s) formation cross-sections (channel 2) at all incident energies (see figures 3 and 4). The most interesting results are accumulated in table 2 and figures 5 and 6. In table 2 and figure 5, we find a comparison between the total H(1s) formation cross-sections,  $\sigma_{12}$ , H(2s) formation cross-sections,  $\sigma_{13}$  (in  $\pi a_0^2$ ) and the available results determined by Ferrante *et al* [7] using the Oppenheimer–Brinkman–Kramer's (OBK) approximation, Daniele



**Figure 6.** Present total hydrogen, H(2s), formation cross-sections ( $\sigma_{13}$  in  $\pi a_0^2$ ) of p–K scattering in comparison with theoretical results [11].

*et al* [8] using Eikonal-approximation treatment and those by Choudhury and Sural [11] using the wave formulation of impulse approximation. Our calculations show that the total cross-sections are considerably lower than those of the compared results at the considered values of the incident energies except at  $k_1^2 = 130$  and  $140$  keV. We find that our values are higher than those of Ferrante *et al* (FBA) [7]. We can also conclude that our results are in good agreement with those of Choudhury and Sural [11] at all considered values of the incident energies between 50 and 500 keV. In table 2 and figure 6, we also find our values of the total H(2s) formation cross-sections,  $\sigma_{13}$  (in  $\pi a_0^2$ ) with those of Choudhury and Sural [11] using the wave formulation of impulse approximation. Our results of the total H(2s) formation cross-sections have the same trend of the compared results and are in reasonable agreement with those of Choudhury and Sural [11] at all considered values of the incident energies. The reason for the difference lies in the different approximations used for the scattering wave function and in neglecting polarization potential effects of the H(1s) formation and H(2s) formation in our calculations. Before leaving this section, it is important to mention that further improvements on the present total collisional cross-sections can also be obtained by considering the effect of polarization potential of H(1s) formation and H(2s) formation atoms and by considering higher excitation channels of H formation in our calculations.

#### 4. Conclusions

Proton–potassium inelastic scattering was studied for the first time using the modified coupled static approximation (three-channel problem). Our interest is focused on H(1s) formation and H(2s) formation atoms in p–K inelastic scattering as a three-channel problem. The present calculations show that the excited hydrogen channel is needed to investigate the collision of the proton with potassium atom. Our values are, in general, lower than the compared results, and we expect that our collisional cross-sections will increase by taking the effect of polarization potentials in our calculations, either by employing a polarized orbital technique or by including pseudopolarization potentials in our calculations. We can also improve our results by considering higher excitation channels of hydrogen formation atom (which are now under consideration by the author).

#### Appendix A: The reactance matrix R

Let us consider the partial wave expansions of the scattering wave functions  $|\psi_1\rangle$ ,  $|\psi_2\rangle$  and  $|\psi_3\rangle$ , that is,

$$\psi_1 = \frac{1}{x} \sum (2\ell + 1) i^\ell f_\ell(x) Y_\ell^0(\hat{x}), \quad (\text{A.1})$$

$$\psi_2 = \frac{1}{\sigma} \sum (2\ell + 1) i^\ell g_\ell(\sigma) Y_\ell^0(\hat{\sigma}) \quad (\text{A.2})$$

and

$$\psi_3 = \frac{1}{\sigma'} \sum (2\ell + 1) i^\ell h_\ell(\sigma') Y_\ell^0(\hat{\sigma}'), \quad (\text{A.3})$$

where  $f_\ell(x)$ ,  $g_\ell(\sigma)$  and  $h_\ell(\sigma')$  are the radial partial wave functions corresponding to the total angular momentum  $\ell$ , of the first, second and third channels, respectively,  $Y_\ell^0(\hat{x})$ ,  $Y_\ell^0(\hat{\sigma})$  and  $Y_\ell^0(\hat{\sigma}')$  are the related spherical harmonics.  $\hat{x}$ ,  $\hat{\sigma}$  and  $\hat{\sigma}'$  are the angles between the vectors  $\vec{x}$ ,  $\vec{\sigma}$  and  $\vec{\sigma}'$ , and the  $z$ -axis.

Substituting eqs (A.1)–(A.3) into eqs (23)–(25), for each value of  $\ell$ , we obtain the following coupled integrodifferential equations:

$$\begin{aligned} & \left[ \frac{d^2}{dx^2} - \frac{\ell(\ell + 1)}{x^2} + k_1^2 \right] f_\ell(x) \\ &= 2\mu_M U_{st}^{(1)}(x) f_\ell(x) \\ &+ \int_0^\infty K_{12}(x, \sigma) g_\ell(\sigma) d\sigma \\ &+ \int_0^\infty K_{13}(x, \sigma') h_\ell(\sigma') d\sigma', \end{aligned} \quad (\text{A.4})$$

$$\begin{aligned} & \left[ \frac{d^2}{d\sigma^2} - \frac{\ell(\ell + 1)}{\sigma^2} + k_2^2 \right] g_\ell(\sigma) \\ &= 2\mu_{M'} U_{st}^{(2)}(\sigma) g_\ell(\sigma) \\ &+ \int_0^\infty K_{21}(\sigma, x) f_\ell(x) dx \\ &+ \int_0^\infty K_{23}(\sigma, \sigma') h_\ell(\sigma') d\sigma' \end{aligned} \quad (\text{A.5})$$

and

$$\begin{aligned} & \left[ \frac{d^2}{d\sigma'^2} - \frac{\ell(\ell + 1)}{\sigma'^2} + k_3^2 \right] h_\ell(\sigma') \\ &= 2\mu_{M''} U_{st}^{(3)}(\sigma') h_\ell(\sigma') \\ &+ \int_0^\infty K_{31}(\sigma', x) f_\ell(x) dx \\ &+ \int_0^\infty K_{32}(\sigma', \sigma) g_\ell(\sigma) d\sigma, \end{aligned} \quad (\text{A.6})$$

where the kernels  $K_{12}$ ,  $K_{13}$ ,  $K_{21}$  and  $K_{31}$  are expanded by

$$\begin{aligned} K_{12}(x, \sigma) &= 2\mu_M (8x\sigma) \iint \Phi_{K(4s)}(r) \Phi_{H(1s)}(\rho) \\ &\times \left[ -\frac{1}{2\mu_{M'}} (\nabla_\sigma^2 + k_2^2) + V_{\text{int}}^{(2)} \right] \\ &\times Y_\ell^0(\hat{x}) Y_\ell^0(\hat{\sigma}) d\hat{x} d\hat{\sigma}, \end{aligned} \quad (\text{A.7})$$

$$K_{13}(x, \sigma') = 2\mu_M(8x\sigma') \iint \Phi_{K(4s)}(r)\Phi_{H(2s)}(\rho') \\ \times \left[ -\frac{1}{2\mu_{M'}}(\nabla_{\sigma'}^2 + k_3^2) + V_{\text{int}}^{(3)} \right] \\ \times Y_\ell^o(\hat{x})Y_\ell^o(\hat{\sigma}')d\hat{x}d\hat{\sigma}', \quad (\text{A.8})$$

$$K_{21}(\sigma, x) = 2\mu_{M'}(8\sigma x) \iint \Phi_{H(1s)}(\rho)\Phi_{K(4s)}(r) \\ \times \left[ -\frac{1}{2\mu_M}(\nabla_x^2 + k_1^2) + V_{\text{int}}^{(1)} \right] \\ \times Y_\ell^o(\hat{x})Y_\ell^o(\hat{\sigma})d\hat{x}d\hat{\sigma} \quad (\text{A.9})$$

and

$$K_{31}(\sigma', x) = 2\mu_{M''}(8\sigma'x) \iint \Phi_{H(2s)}(\rho')\Phi_{K(4s)}(r) \\ \times \left[ -\frac{1}{2\mu_M}(\nabla_x^2 + k_1^2) + V_{\text{int}}^{(1)} \right] \\ \times Y_\ell^o(\hat{x})Y_\ell^o(\hat{\sigma}')d\hat{x}d\hat{\sigma}' \quad (\text{A.10})$$

and the kernels  $K_{23}(\sigma, \sigma')$  and  $K_{32}(\sigma', \sigma)$  are equal to zero due to the orthogonality of the wave functions of the ground and excited states of hydrogen. (The number eight appearing in the preceding equations refers to the Jacobians of the transformations  $\int dr \rightarrow 8 \int d\sigma$  and  $\int d\rho \rightarrow 8 \int dx$ .)

Let us now rewrite eqs (A.4)–(A.6) as

$$\left[ \frac{d^2}{dx^2} - \frac{\ell(\ell+1)}{x^2} + k_1^2 \right] f_\ell(x) = 2\mu_M U_{st}^{(1)}(x)f_\ell(x) \\ + Q_1(x) + Q_3(x), \quad (\text{A.11})$$

$$\left[ \frac{d^2}{d\sigma^2} - \frac{\ell(\ell+1)}{\sigma^2} + k_2^2 \right] g_\ell(\sigma) = 2\mu_{M'} U_{st}^{(2)}(\sigma)g_\ell(\sigma) \\ + Q_2(\sigma) \quad (\text{A.12})$$

and

$$\left[ \frac{d^2}{d\sigma'^2} - \frac{\ell(\ell+1)}{\sigma'^2} + k_3^2 \right] h_\ell(\sigma') = 2\mu_{M''} U_{st}^{(3)}(\sigma') \\ \times h_\ell(\sigma') + Q_5(\sigma'), \quad (\text{A.13})$$

where

$$Q_1(x) = \int_0^\infty K_{12}(x, \sigma)g_\ell(\sigma)d\sigma, \quad (\text{A.14})$$

$$Q_3(x) = \int_0^\infty K_{13}(x, \sigma')h_\ell(\sigma')d\sigma', \quad (\text{A.15})$$

$$Q_2(\sigma) = \int_0^\infty K_{21}(\sigma, x)f_\ell(x)dx, \quad (\text{A.16})$$

and

$$Q_5(\sigma') = \int_0^\infty K_{31}(\sigma', x)f_\ell(x)dx. \quad (\text{A.17})$$

The three coupled integrodifferential (scattering) equations (A.11)–(A.13) are identical with the inhomogeneous equation

$$[\varepsilon - H_0(u)]|\xi(u)\rangle = |\zeta(u)\rangle, \quad (\text{A.18})$$

where

$u = x$  implies:

$$\varepsilon = k_1^2, \quad H_0(x) = -\frac{d}{dx^2} + \frac{\ell(\ell+1)}{x^2},$$

$$|\xi(x)\rangle = f_\ell(x),$$

$$|\zeta(x)\rangle = 2\mu_M U_{st}^{(1)}(x)f_\ell(x) + Q_1(x) + Q_3(x),$$

$u = \sigma$  implies:

$$\varepsilon = k_2^2, \quad H_0(\sigma) = -\frac{d}{d\sigma^2} + \frac{\ell(\ell+1)}{\sigma^2},$$

$$|\xi(\sigma)\rangle = g_\ell(\sigma),$$

$$|\zeta(\sigma)\rangle = 2\mu_{M'} U_{st}^{(2)}(\sigma)g_\ell(\sigma) + Q_2(\sigma)$$

and

$u = \sigma'$  implies:

$$\varepsilon = k_3^2, \quad H_0(\sigma') = -\frac{d}{d\sigma'^2} + \frac{\ell(\ell+1)}{\sigma'^2},$$

$$|\xi(\sigma')\rangle = h_\ell(\sigma'),$$

$$|\zeta(\sigma')\rangle = 2\mu_{M''} U_{st}^{(3)}(\sigma')h_\ell(\sigma') + Q_5(\sigma').$$

The formal solutions of eq. (A.18) is given by the Lippmann–Schwinger equation

$$|\xi\rangle = |\xi_0\rangle + G_0|\zeta\rangle, \quad (\text{A.19})$$

where  $G_0$  is the Green operator  $(\varepsilon - H_0)^{-1}$  and  $|\xi_0\rangle$  is the solution of the homogeneous equation

$$(\varepsilon - H_0)|\xi_0\rangle = |0\rangle. \quad (\text{A.20})$$

The partial-wave expansion of  $G_0$  in the three channels enables us to write the formal solution of (A.11)–(A.13) as

$$f_\ell^{(i)}(x) = \left\{ \delta_{i1} + \frac{1}{k_1} \int_0^\infty \tilde{g}_\ell(k_1 x') [2\mu_M U_{st}^{(1)}(x')f_\ell^{(i)}(x') \right. \\ \left. + Q_1^{(i)}(x') + Q_3^{(i)}(x')] dx' \right\}_1 \tilde{f}_\ell(k_1 x)$$

$$\begin{aligned}
 & + \left\{ -\frac{1}{k_1} \int_0^\infty \tilde{f}_\ell(k_1 x') [2\mu_M U_{st}^{(1)}(x') f_\ell^{(i)}(x')] \right. \\
 & \left. + Q_1^{(i)}(x') + Q_3^{(i)}(x') \right] dx' \Big\}_2 \tilde{g}_\ell(k_1 x), \\
 & i = 1, 2, 3 \tag{A.21}
 \end{aligned}$$

$$\begin{aligned}
 g_\ell^{(i)}(\sigma) & = \left\{ \delta_{i2} + \frac{1}{k_2} \int_0^\infty \tilde{g}_\ell(k_2 \sigma') [2\mu_{M'} U_{st}^{(2)}(\sigma') g_\ell^{(i)}(\sigma')] \right. \\
 & \left. + Q_2^{(i)}(\sigma') \right] d\sigma' \Big\}_3 \tilde{f}_\ell(k_2 \sigma) \\
 & + \left\{ -\frac{1}{k_2} \int_0^\infty \tilde{f}_\ell(k_2 \sigma') [2\mu_{M'} U_{st}^{(2)}(\sigma') g_\ell^{(i)}(\sigma')] \right. \\
 & \left. + Q_2^{(i)}(\sigma') \right] d\sigma' \Big\}_4 \tilde{g}_\ell(k_2 \sigma), \quad i = 1, 2, 3 \tag{A.22}
 \end{aligned}$$

and

$$\begin{aligned}
 h_\ell^{(i)}(\sigma') & = \left\{ \delta_{i3} + \frac{1}{k_3} \int_0^\infty \tilde{g}_\ell(k_3 \sigma'') [2\mu_{M''} U_{st}^{(3)}(\sigma'') h_\ell^{(i)}(\sigma'')] \right. \\
 & \left. + Q_5^{(i)}(\sigma'') \right] d\sigma'' \Big\}_5 \tilde{f}_\ell(k_3 \sigma') \\
 & + \left\{ -\frac{1}{k_3} \int_0^\infty \tilde{f}_\ell(k_3 \sigma'') [2\mu_{M''} U_{st}^{(3)}(\sigma'') h_\ell^{(i)}(\sigma'')] \right. \\
 & \left. + Q_5^{(i)}(\sigma'') \right] d\sigma'' \Big\}_6 \tilde{g}_\ell(k_3 \sigma'), \quad i = 1, 2, 3, \tag{A.23}
 \end{aligned}$$

where the delta functions  $\delta_{ij}$ ,  $i, j = 1, 2, 3$ , specify two independent forms of solutions for each of  $f_\ell(x)$ ,  $g_\ell(\sigma)$  and  $h_\ell(\sigma')$  in channels  $i = 1, 2, 3$  according to the channel considered. Thus, if  $i = 1$ , the first element in the  $\{ \}$  bracket of  $f_\ell(x)$ , for example, will be 1 defining the first form of solution. For  $i = 2, 3$  this element will be zero defining the second form. The functions  $\tilde{f}_\ell(\eta)$  and  $\tilde{g}_\ell(\eta)$ ,  $\eta = k_1 x, k_2 \sigma$  or  $k_3 \sigma'$ , are related to the Bessel functions of the first and second channels, that is,  $j_\ell(\eta)$  and  $y_\ell(\eta)$ , respectively, by the relations  $\tilde{f}_\ell(\eta) = \eta j_\ell(\eta)$  and  $\tilde{g}_\ell(\mu) = -\eta y_\ell(\eta)$ .

It is obvious from eqs (A.21)–(A.23) that the solutions can be only found iteratively and the  $\nu$ th iterations are calculated by

$$\begin{aligned}
 f_\ell^{(i,\nu)}(x) & = \left\{ \delta_{i1} + \frac{1}{k_1} \int_0^X \tilde{g}_\ell(k_1 x') [2\mu_M U_{st}^{(1)}(x')] \right. \\
 & \left. \times f_\ell^{(i,\nu)}(x') + Q_1^{(i,\nu-1)}(x') \right. \\
 & \left. + Q_3^{(i,\nu-1)}(x') \right] dx' \Big\}_1 \tilde{f}_\ell(k_1 x)
 \end{aligned}$$

$$\begin{aligned}
 & + \left\{ -\frac{1}{k_1} \int_0^X \tilde{f}_\ell(k_1 x') [2\mu_M U_{st}^{(1)}(x') f_\ell^{(i,\nu)}(x')] \right. \\
 & \left. + Q_1^{(i,\nu-1)}(x') + Q_3^{(i,\nu-1)}(x') \right] dx' \Big\}_2 \tilde{g}_\ell(k_1 x), \\
 & i = 1, 2, 3; \quad \nu \geq 1, \tag{A.24}
 \end{aligned}$$

$$\begin{aligned}
 g_\ell^{(i,\nu)}(\sigma) & = \left\{ \delta_{i2} + \frac{1}{k_2} \int_0^\Sigma \tilde{g}_\ell(k_2 \sigma') \right. \\
 & \left. \times [2\mu_{M'} U_{st}^{(2)}(\sigma') g_\ell^{(i,\nu)}(\sigma')] \right. \\
 & \left. + Q_2^{(i,\nu)}(\sigma') \right] d\sigma' \Big\}_3 \tilde{f}_\ell(k_2 \sigma) \\
 & + \left\{ -\frac{1}{k_2} \int_0^\Sigma \tilde{f}_\ell(k_2 \sigma') \right. \\
 & \left. \times [2\mu_{M'} U_{st}^{(2)}(\sigma') g_\ell^{(i,\nu)}(\sigma')] \right. \\
 & \left. + Q_2^{(i,\nu)}(\sigma') \right] d\sigma' \Big\}_4 \tilde{g}_\ell(k_2 \sigma), \\
 & i = 1, 2, 3; \quad \nu \geq 0 \tag{A.25}
 \end{aligned}$$

and

$$\begin{aligned}
 h_\ell^{(i,\nu)}(\sigma') & = \left\{ \delta_{i3} + \frac{1}{k_3} \int_0^{\Sigma'} \tilde{g}_\ell(k_3 \sigma'') \right. \\
 & \left. \times [2\mu_{M''} U_{st}^{(3)}(\sigma'') h_\ell^{(i,\nu)}(\sigma'')] \right. \\
 & \left. + Q_5^{(i,\nu)}(\sigma'') \right] d\sigma'' \Big\}_5 \tilde{f}_\ell(k_3 \sigma') \\
 & + \left\{ -\frac{1}{k_3} \int_0^{\Sigma'} \tilde{f}_\ell(k_3 \sigma'') \right. \\
 & \left. \times [2\mu_{M''} U_{st}^{(3)}(\sigma'') h_\ell^{(i,\nu)}(\sigma'')] \right. \\
 & \left. + Q_5^{(i,\nu)}(\sigma'') \right] d\sigma'' \Big\}_6 \tilde{g}_\ell(k_3 \sigma'), \\
 & i = 1, 2, 3; \quad \nu \geq 0. \tag{A.26}
 \end{aligned}$$

The zeroth iteration of  $f_\ell^{(i,0)}(x)$  is obtained by

$$\begin{aligned}
 f_\ell^{(i,0)}(x) & = \left\{ \delta_{i1} + \frac{1}{k_1} \int_0^X \tilde{g}_\ell(k_1 x') \right. \\
 & \left. \times [2\mu_M U_{st}^{(1)}(x') f_\ell^{(i,0)}(x')] \right] dx' \Big\}_1 \tilde{f}_\ell(k_1 x) \\
 & + \left\{ -\frac{1}{k_1} \int_0^X \tilde{f}_\ell(k_1 x') \right. \\
 & \left. \times [2\mu_M U_{st}^{(1)}(x') f_\ell^{(i,0)}(x')] \right] dx' \Big\}_2 \tilde{g}_\ell(k_1 x), \\
 & i = 1, 2, 3, \tag{A.27}
 \end{aligned}$$

where  $X$ ,  $\Sigma$  and  $\Sigma'$  specify the integration range away from the nucleus over which the integrals at eqs (A.24)–(A.27) are calculated using Simpson's expansions. The functions  $Q_1^{(i,\nu-1)}(x')$ ,  $Q_3^{(i,\nu-1)}(x')$ ,

$Q_2^{(i,v)}(\sigma)$  and  $Q_5^{(i,v)}(\sigma')$ , in eqs (A.24)–(A.26), are now defined by

$$Q_1^{(i,v-1)}(x') = \int_0^{\Sigma} K_{12}(x', \sigma) g_\ell^{(i,v-1)}(\sigma) d\sigma, \quad (\text{A.28})$$

$$Q_3^{(i,v-1)}(x') = \int_0^{\Sigma'} K_{13}(x', \sigma') h_\ell^{(i,v-1)}(\sigma') d\sigma', \quad (\text{A.29})$$

$$Q_2^{(i,v)}(\sigma') = \int_0^X K_{21}(\sigma', x) f_\ell^{(i,v)}(x) dx \quad (\text{A.30})$$

and

$$Q_5^{(i,v)}(\sigma'') = \int_0^X K_{31}(\sigma'', x) f_\ell^{(i,v)}(x) dx. \quad (\text{A.31})$$

To find the starting value of  $f_\ell^{(i,0)}(x)$ , we consider the Taylor expansion of  $U_{st}^{(1)}(x)$ ,  $\tilde{f}_\ell(k_1x)$  and  $\tilde{g}_\ell(k_1x)$  around the origin (see Appendix B).

Equations (A.24)–(A.26) can be abbreviated to

$$f_\ell^{(i,v)}(x) = a_1^{(i,v)} \tilde{f}_\ell(k_1x) + b_1^{(i,v)} \tilde{g}_\ell(k_1x), \quad (\text{A.32})$$

$$i = 1, 2, 3,$$

$$g_\ell^{(i,v)}(\sigma) = a_2^{(i,v)} \tilde{f}_\ell(k_2\sigma) + b_2^{(i,v)} \tilde{g}_\ell(k_2\sigma), \quad (\text{A.33})$$

$$i = 1, 2, 3$$

and

$$h_\ell^{(i,v)}(\sigma') = a_3^{(i,v)} \tilde{f}_\ell(k_3\sigma') + b_3^{(i,v)} \tilde{g}_\ell(k_3\sigma'), \quad (\text{A.34})$$

$$i = 1, 2, 3,$$

where

$$a_1^{(i,v)} = \{ \}_1, \quad b_1^{(i,v)} = \{ \}_2, \quad a_2^{(i,v)} = \{ \}_3,$$

$$b_2^{(i,v)} = \{ \}_4, \quad a_3^{(i,v)} = \{ \}_5, \quad b_3^{(i,v)} = \{ \}_6,$$

and the preceding six brackets are the coefficients of eqs (A.24)–(A.26).

The coefficients at eqs (A.32)–(A.34) are elements of the following matrices:

$$a^v = \begin{pmatrix} \sqrt{2\mu_M/k_1} a_1^{(1,v)} & \sqrt{2\mu_M/k_1} a_1^{(2,v)} & \sqrt{2\mu_M/k_1} a_1^{(3,v)} \\ \sqrt{2\mu_M/k_2} a_2^{(1,v)} & \sqrt{2\mu_M/k_2} a_2^{(2,v)} & \sqrt{2\mu_M/k_2} a_2^{(3,v)} \\ \sqrt{2\mu_{M'}/k_3} a_3^{(1,v)} & \sqrt{2\mu_{M'}/k_3} a_3^{(2,v)} & \sqrt{2\mu_{M'}/k_3} a_3^{(3,v)} \end{pmatrix} \quad (\text{A.35})$$

and

$$b^v = \begin{pmatrix} \sqrt{2\mu_M/k_1} b_1^{(1,v)} & \sqrt{2\mu_M/k_1} b_1^{(2,v)} & \sqrt{2\mu_M/k_1} b_1^{(3,v)} \\ \sqrt{2\mu_{M'}/k_2} b_2^{(1,v)} & \sqrt{2\mu_{M'}/k_2} b_2^{(2,v)} & \sqrt{2\mu_{M'}/k_2} b_2^{(3,v)} \\ \sqrt{2\mu_{M'}/k_3} b_3^{(1,v)} & \sqrt{2\mu_{M'}/k_3} b_3^{(2,v)} & \sqrt{2\mu_{M'}/k_3} b_3^{(3,v)} \end{pmatrix} \quad (\text{A.36})$$

which are connected with the reactance matrix,  $R^v$ , through the relation

$$\{R^v\}_{ij} = \{b^v(a^v)^{-1}\}_{ij}. \quad (\text{A.37})$$

## Appendix B: The numerical iterative method

This appendix contains a brief discussion of the iteration procedure used for calculating the elements of the reactance matrix. This has been achieved using eqs (A.24)–(A.26) where  $X$ ,  $\Sigma$  and  $\Sigma'$  represent the ranges of integrations over  $x$ ,  $\sigma$  and  $\sigma'$ , respectively. Physically,  $X$  ( $X = nh$ , where  $n$  is the number of mesh points and  $h$  is the Simpson step, or mesh size), represents the distance at which we assume that the scattered protons are not affected by the potassium atoms,  $\Sigma$  ( $= nh$ ) is the distance at which the ground-state hydrogen atom and the proton of the target are totally separated and  $\Sigma'$  ( $= nh$ ) is the distance at which the excited hydrogen atom and the proton of the target are totally separated.

To calculate the integrals in eqs (A.24)–(A.31) we use Simpson's rule. Thus, we expand  $Q_1^{(i,v-1)}(x)$ ,  $Q_3^{(i,v-1)}(x)$ ,  $Q_2^{(i,v)}(\sigma)$  and  $Q_5^{(i,v)}(\sigma')$  at point  $q$  of the configuration space as follows:

$$Q_1^{(i,v-1)}(x_q) = \sum_{p=1}^n \{ \omega_p^{(1)} K_{12}^{(1)}(\sigma_p, x_q) + \omega_p^{(2)} K_{12}^{(2)}(\sigma_p, x_q) + \omega_p^{(3)} K_{12}^{(3)}(\sigma_p, x_q) \} g_\ell^{(i,v-1)}(\sigma_p), \quad (\text{B.1})$$

$$v \geq 1,$$

$$Q_3^{(i,v-1)}(x_q) = \sum_{p=1}^n \{ \omega_p^{(1)} K_{13}^{(1)}(\sigma'_p, x_q) + \omega_p^{(2)} K_{13}^{(2)}(\sigma'_p, x_q) + \omega_p^{(3)} K_{13}^{(3)}(\sigma'_p, x_q) \} h_\ell^{(i,v-1)}(\sigma'_p), \quad (\text{B.2})$$

$$v \geq 1,$$

$$Q_2^{(i,v)}(\sigma_q) = \sum_{p=1}^n \{ \omega_p^{(1)} K_{21}^{(1)}(\sigma_q, x_p) + \omega_p^{(2)} K_{21}^{(2)}(\sigma_q, x_p) + \omega_p^{(3)} K_{21}^{(3)}(\sigma_q, x_p) \} f_\ell^{(i,v)}(x_p), \quad (\text{B.3})$$

$$v \geq 0,$$

and

$$Q_5^{(i,v)}(\sigma'_q) = \sum_{p=1}^n \{ \omega_p^{(1)} K_{31}^{(1)}(\sigma'_q, x_p) + \omega_p^{(2)} K_{31}^{(2)}(\sigma'_q, x_p) + \omega_p^{(3)} K_{31}^{(3)}(\sigma'_q, x_p) \} f_\ell^{(i,v)}(x_p), \quad (\text{B.4})$$

$$v \geq 0,$$

where  $\omega_p^{(1)}$ 's are the usual Simpson weights ( $h/3, 4h/3, 2h/3, \dots, 2h/3, 4h/3, h/3$ ) and  $\omega_p^{(2)}$ 's,  $\omega_p^{(3)}$ 's are modified weights used for avoiding the singularities (see refs [14,15]). The variables  $x_p, \sigma_p$  and  $\sigma'_p$  are chosen such that  $x_p = \sigma_p = \sigma'_p = ph, p = 1, 2, \dots, n$ .

An essential point in the determination of the integrals in eqs (A.24)–(A.31) is the calculation of the starting values of the functions  $f_\ell^{(i,v)}(x), g_\ell^{(i,v)}(\sigma)$  and  $h_\ell^{(i,v)}(\sigma')$ , that is, their values at  $x_p = \sigma_p = \sigma'_p = h$ , respectively, which is determined as follows (note that  $f_\ell^{(i,v)}(0) = g_\ell^{(i,v)}(0) = h_\ell^{(i,v)}(0) = 0$ ).

Considering the Taylor expansion of  $U_{st}^{(1)}(r), \tilde{f}_\ell(kr)$  and  $\tilde{g}_\ell(kr)$  around the origin, we obtain

$$U_{st}^{(1)}(x) \approx 2 \left( \frac{Z}{x} + D_0 + D_1x + \dots \right), \tag{B.5}$$

where  $Z = 1, D_0$  and  $D_1$  are constants, and

$$\tilde{f}_\ell(k_1x) \cong \frac{(k_1x)^{\ell+1}}{(2\ell+1)!!} \left[ 1 - \frac{(k_1x)^2/2}{1!(2\ell-1)} + \frac{(k_1x)^4/4}{2!(2\ell+3)(2\ell+5)} + \dots \right] \tag{B.6}$$

and

$$\tilde{g}_\ell(k_1x) \cong \frac{(2\ell+1)!!}{(2\ell+1)(k_1x)^\ell} \left[ 1 + \frac{(k_1x)^2/2}{1!(2\ell-1)} + \frac{(k_1x)^4/4}{2!(2\ell-1)(3\ell-2)} + \dots \right]. \tag{B.7}$$

Assume that  $f_\ell^{(i,0)}(x)$  behaves close to the origin as

$$f_\ell^{(i,0)}(x) \cong C_1x^{\ell+1} + C_2x^{\ell+2} + C_3x^{\ell+3} + C_4x^{\ell+4} + \dots \tag{B.8}$$

Substituting eqs (B.5)–(B.8) into eq. (A.27) yields

$$\left. \begin{aligned} C_1 &= \frac{k^{\ell+1}}{(2\ell+1)!!}, \quad C_2 = \frac{Z}{\ell+1}C_1, \\ C_3 &= \left[ \frac{D_0}{2\ell+3} + \frac{Z^2}{(\ell+1)(2\ell+3)} - \frac{k^2}{2(2\ell-1)} \right] C_1 \\ C_4 &= \{ \Omega_1[C_1\Omega_4D_1 + C_1\Omega_5Z + D_0\Omega_4C_2 \\ &\quad + C_3\Omega_4Z]/3 + \Omega_2\Omega_4C_1Z \\ &\quad - \Omega_4[C_1\Omega_1D_1 + C_1\Omega_2Z + C_2\Omega_1D_0 \\ &\quad + C_3\Omega_1Z]/(2\ell+4) \\ &\quad - \Omega_1\Omega_5C_1Z/(2\ell+2) \} / k, \end{aligned} \right\} \tag{B.9}$$

where

$$\left. \begin{aligned} \Omega_1 &= \frac{k^{\ell+1}}{(2\ell+1)!!}, \quad \Omega_2 = \frac{-k^{\ell+3}}{2(2\ell-1)(2\ell+1)!!}, \\ \Omega_3 &= \frac{k^{\ell+5}}{8(2\ell+3)(2\ell+5)(2\ell+1)!!} \\ \Omega_4 &= \frac{(2\ell+1)!!}{(2\ell+1)k^\ell}, \quad \Omega_5 = \frac{(2\ell+1)!!}{2(2\ell-1)(2\ell+1)k^{\ell-2}}, \\ \Omega_6 &= \frac{(2\ell+1)!!}{8(2\ell+1)(2\ell-1)(3\ell-2)k^{\ell-4}}. \end{aligned} \right\} \tag{B.10}$$

Introducing constants  $C_1, C_2, C_3$  and  $C_4$  into eq. (B.8) and setting  $x = h$  (the interval of integration), we obtain a starting value  $f_\ell^{(i,0)}(x)$  (note that the first four terms of eq. (B.8) are enough for obtaining a good starting value specially when  $h$  is reasonably small). The above procedure can also be applied for calculating the starting value of  $g_\ell^{(i,v)}(\sigma)$  and  $h_\ell^{(i,v)}(\sigma)$  at different values of  $\ell, i$  and  $v$ .

The iteration process starts by introducing  $f_\ell^{(i,0)}(x), i = 1, 2, 3$  values into eqs (A.30) and (A.31) to find  $Q_2^{(i,0)}(\sigma')$  and  $Q_5^{(i,0)}(\sigma'')$ , which can be used in the right-hand side of eqs (A.25) and (A.26) to obtain  $g_\ell^{(i,0)}(\sigma)$  and  $h_\ell^{(i,0)}(\sigma')$ . The values of the last quantities can be introduced into eqs (A.28) and (A.29) to calculate  $Q_1^{(i,0)}(x')$  and  $Q_3^{(i,0)}(x')$ , which may be employed in eq. (A.24) for determining  $f_\ell^{(i,1)}(x)$ . This iteration process can be repeated as many times as we need and the judge of its quantity is the stationary variation of the elements of the reactance matrix  $R_{ij}^\nu$  where  $\nu$  increase.

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