



Brazilian Journal of Physics

ISSN: 0103-9733

luizno.bjp@gmail.com

Sociedade Brasileira de Física
Brasil

Elkilany, S. A.

Effect of Polarization Potential on Proton–Sodium Inelastic Scattering

Brazilian Journal of Physics, vol. 44, núm. 6, 2014, pp. 629-637

Sociedade Brasileira de Física

São Paulo, Brasil

Available in: <http://www.redalyc.org/articulo.oa?id=46432477004>

- How to cite
- Complete issue
- More information about this article
- Journal's homepage in redalyc.org

redalyc.org

Scientific Information System

Network of Scientific Journals from Latin America, the Caribbean, Spain and Portugal

Non-profit academic project, developed under the open access initiative

Effect of Polarization Potential on Proton–Sodium Inelastic Scattering

S. A. Elkilany

Received: 15 June 2014 / Published online: 22 October 2014
© Sociedade Brasileira de Física 2014

Abstract Inelastic collisions of protons with sodium atoms are treated for the first time within the framework of the coupled static and frozen core approximations. The method is used for calculating partial and total cross-sections with the assumption that only two channels (elastic and hydrogen formation in 2s-state) are open. The calculations are carried out, in each case, for seven values of the total angular momentum ℓ ($0 \leq \ell \leq 6$). In the second channel, the effect of “switching on” the polarization potential of hydrogen (in 2s-state) on the coupled static cross-sections is investigated. Although the resulting hydrogen (in 2s-state) formation cross-sections are smaller than the elastic ones, their large values should draw the attention of experimental and theoretical physicists to the field of proton–alkali atom collisions. Our results for the total hydrogen (2s-state) formation cross-sections and those determined by previous authors are in reasonable agreement.

Keywords Inelastic scattering · Proton · Excited hydrogen · Sodium

PACS Nos 34.80.Dp · 34.80.Gs · 34.80.Ht

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 femtosecond laser has tremendously enhanced the experimental identification of these states in chemical and physical reactions [1]. Theoretical investigation of proton–atom scattering is given by many authors. Most theoretical treatments of proton–atom are based on calculations of differential, partial, and total cross-sections as functions of the incident energy, using different approximations. Banyard and Shirtcliffe [2] used the continuum-distorted wave (CDW) method to calculate cross-sections for electron capture by fast protons from the lithium atom and its related positive ions. Each target electronic state is described by a Hartree-Fock wave function. Results for the individual capture states ($n\ell$) are also reported for the Li^+ target. For the lithium atom, capture can occur from either the K or the L shell. A procedure for determining the effective screening of the target nucleus by the uncaptured “passive” electrons is discussed, and the sensitivity of the cross-sections with respect to such screening is examined. Ferrante et al. [3] reported the capture cross-sections into ground and excited hydrogen states by protons colliding with alkali atoms. By means of simple models, the capture of both valence and core electrons is considered. The OBK approximation is used, and the alkali atom is treated in a one-electron picture. The treatment of the core electron capture given for proton–alkali atom collisions is expected to be equally suitable for any kind of many-electron target atoms. Daniele et al. [4] applied the eikonal approximation treatment developed previously within the framework of the time-dependent impact parameter method for high-energy proton–alkali atom charge transfer to calculate total cross-sections of valence electron into the hydrogen atom ground state from the whole series of the alkali atoms. The latter is treated as one-electron model atoms by means of very simple model potentials and wave functions. The calculated cross-sections are found to be lower than the OBK and the FBA results. Ferrante and Fiordilino [5] treated high-energy proton–alkali atom charge exchange in the eikonal approximation within the

S. A. Elkilany (✉)
Department of Mathematics, Faculty of Science, Kafrelsheikh
University, Kafrelsheikh, Egypt
e-mail: sabbelkilany@yahoo.com

S. A. Elkilany
Department of Mathematics, Faculty of Science, Ad Damman
University, Dammam, Kingdom of Saudi Arabia

framework of the well-known time-dependent semi-classical parameter method. Detailed calculations are specialized to the proton–lithium atom charge exchange, for which the total cross-section is obtained in closed form. Fritsch and Lin [6] used a modified two-center atomic orbital expansion in an investigation of electron capture in collisions of H^+ and He^{2+} ions with lithium atoms. Total capture cross-sections are found to agree with experimental data wherever the measurements have led to a consistent picture among themselves. Choudhury and Sural [7] applied the wave formulation of the impulse approximation to the case of electron capture into the ground, 2s, and 2p excited states of hydrogen in collisions between protons and alkali-metal atoms sodium, potassium, rubidium, and cesium. The transition matrix elements have been numerically calculated and used to determine the differential and integral cross-sections for charge transfer for incident energy varying between 50 and 500 keV. Tiwari [8] investigated the differential and total cross-sections in the formation of H atom in the 2s excited state of proton–lithium and proton–sodium scattering by using the Coulomb-projected Born (CPB) approximation in the energy range from 50 to 10,000 keV. The results thus obtained are compared with the available results and found to be in reasonable agreement. Elkilany and Abdel-Raouf [9] investigated the effect of switching on various polarization potentials on antiproton–positronium inelastic collisions in detail within the framework of the coupled static model and compared their results with available results. Elkilany [10] used coupled static approximation and Green's function iterative numerical technique for calculating partial and total cross-sections for antiproton–positronium inelastic scattering corresponding to seven values of the total angular momentum ℓ ($0 \leq \ell \leq 6$). It is assumed that elastic and antihydrogen formation channels are open. The effect of switching on various polarization potentials on antiproton–positronium inelastic scattering is investigated in detail. Elkilany [11] employed an elaborate coupled static formalism for the treatment of proton–lithium collisions at wide range of incident energies, between 10 and 1000 keV. Only elastic and formation of excited hydrogen, H(2s), channels are considered. Polarization potential of lithium atom is taken into consideration in calculating the corresponding total cross-section.

Our investigation of p–Li inelastic scattering showed that hydrogen formation in 2s-state, H(2s), plays an important role in the total collisional cross-sections. In the present work, we present the first treatment of the inelastic collisions of proton by sodium atoms. The importance of this scattering problem is twofold: (1) The target is easy to prepare experimentally and (2) it possesses valence electron with lower binding energy and core electrons with large polarizability (a fact which leads to interesting features in the rearrangement cross-sections). The effects of switching on polarization potential on p–Na inelastic collisions are investigated in detail within the framework of the coupled static model. The

iterative Green's function partial wave expansion technique was used. The next section contains a brief presentation of our mathematical formalism, Section 3 is devoted to the discussion of our results, and in Section 4, we give the conclusion on the results which we obtained in the present work. The Appendix involves a short treatment of the method of obtaining the reactance matrix that is used for calculating the partial and the total cross-sections.

2 Theoretical Formalism

The two channel scattering problems under investigation can be sketched by:

$$p + Na(3s) = \begin{cases} p + Na(3s) & \text{(Elastic channel)} \\ H(2s) + Na^+ & \text{(H(2s) formation channel)} \end{cases} \quad (1)$$

The one valence electron model of an alkali target (Na) is described (in Rydberg units) by the Hamiltonian [12]:

$$H_{Na(3s)} = -\frac{1}{2\mu_m} \nabla_r^2 - \frac{2}{r} + V_c(r) \quad (2)$$

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

$$V_c(r) = V_{cCoul}(r) + V_{cex}(r) \quad (3)$$

where $V_{cCoul}(r)$ and $V_{cex}(r)$ are the Coulomb and exchange parts of the core potential.

Following Clementi and Roetti [13], the wave function of the i th electron in the orbital j of the target is expanded as,

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

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

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

Above, k_{jp} are integers or zero, A_{jp} are normalization factors given by

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

and the spherical harmonics Y_{jp} are normalized by $\langle Y_{jp}(\vartheta_i, \phi_i) | Y_{jp}(\vartheta_i, \phi_i) \rangle = 1$. The constants c_{jp} and α_{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:

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

In Eq. (4) and Eq. (7) m_j 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:

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

where M is the number of orbitals and N_j is the number of electrons occupying the orbital j . The prime on the sum sign means that the term $-2/r$ is repeated for each j . The exchange part of the core potential is defined by

$$V_{\text{cex}}(r) = - \sum_{j=1}^M \langle \Phi_{\text{Na}(3s)}(r_i) | \frac{2}{|r-r_i|} | \Phi_j(r_i) \rangle \quad (9)$$

where the subscript Na(3s) 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:

$$E_{\text{Na}(3s)} = - \langle \Phi_{\text{Na}(3s)}(r) | H_{\text{Na}(3s)} | \Phi_{\text{Na}(3s)}(r) \rangle \quad (10)$$

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

$$H = H^{(1)} = H_T - \frac{1}{2\mu_M} \nabla_x^2 + V_{\text{int}}^{(1)}, \quad (11)$$

where μ_M is the reduced mass of first channel and $V_{\text{int}}^{(1)}$ denotes the interaction between the incident proton and target atom, i.e., (see Fig. 1)

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

Where

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

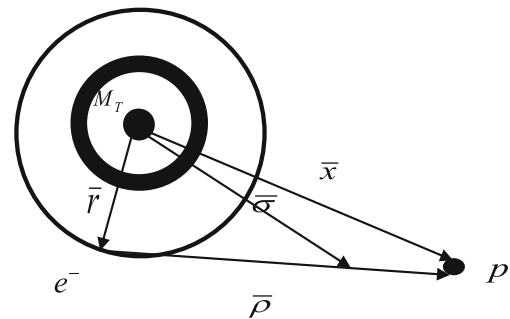


Fig. 1 \bar{x} is the position vector of projectile proton with respect to the center of mass of the target, \bar{r} is the position vector of the valence electron of target with respect to center of mass of the target, $\bar{\rho}$ is the position vector of projectile proton with respect to the valence electron of the target, $\bar{\sigma}$ is the position vector of the center of mass of H(2s) from the target, M_T is the mass of the target

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

$$E = E^{(1)} = E_{\text{Na}(3s)} + \frac{1}{2\mu_M} k_1^2, \quad (14)$$

$\frac{1}{2\mu_M} k_1^2$ is the kinetic energy of the incident proton relative to target nucleus.

The total Hamiltonian of the second channel, H(2s) formation, is expressed (in Rydberg units and frozen core approximation) as:

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

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

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

and the total energy of the second channel is determined by:

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

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

$$\frac{k_2^2}{2\mu_{M'}} = \left(E_{\text{Na}(3s)} + \frac{1}{2\mu_M} k_1^2 - E_{\text{H}(2s)} \right) \quad (18)$$

where $E_{H(2s)} = -0.25$ Ryd is the energy of the first 2s excited state of H and $\frac{k_2^2}{2\mu_M} > 0$ means that H(2s) channel is open. Otherwise, it is closed. Thus, H(2s) formation is only possible if $k_1^2 > 2\mu_M(E_{H(2s)} - E_{Na(3s)})$.

The coupled static approximation states that the solution of the two channel scattering problem under consideration is subjected to the following conditions [14]:

$$\langle \Phi_{Na(3s)} | H - E | \Psi \rangle = 0, \quad (19)$$

$$\langle \Phi_{H(2s)} | H - E | \Psi \rangle = 0 \quad (20)$$

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

$$|\Psi\rangle = |\Phi_{Na(3s)}(r)\rangle |\psi_1(x)\rangle + |\Phi_{H(2s)}(\rho)\rangle |\psi_2(\sigma)\rangle \quad (21)$$

where

$$\Phi_{H(2s)} = \frac{1}{\sqrt{32\pi}} (2-\rho) \exp(-\rho/2) \quad (22)$$

is the ground state wave function of H(2s), $\psi_1(x)$ is the wave function describing the scattered protons, and $\psi_2(x)$ is the scattering wave function of the second channel. Substituting Eq. (14) and Eq. (21) in Eq. (19), we obtain:

$$\frac{1}{2\mu_M} (\nabla_x^2 + k_1^2) |\psi_1\rangle = U_{st}^{(1)}(x) |\psi_1\rangle + \langle \Phi_{Na(3s)} | H^{(2)} - E^{(2)} | \Phi_{H(2s)} \psi_2 \rangle, \quad (23)$$

Substituting Eq. (17) and Eq. (21) in Eq. (20), we obtain:

$$\frac{1}{2\mu_M} (\nabla_\sigma^2 + k_2^2) |\psi_2\rangle = U_{st}^{(2)}(\sigma) |\psi_2\rangle + \langle \Phi_{H(2s)} | H^{(1)} - E^{(1)} | \Phi_{Na(3s)} \psi_1 \rangle \quad (24)$$

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

$$U_{st}^{(1)}(x) = \langle \Phi_{Na(3s)}(r) | V_{int}^{(1)} | \Phi_{Na(3s)}(r) \rangle \quad (25)$$

$$U_{st}^{(2)}(\sigma) = \langle \Phi_{H(2s)}(\rho) | V_{int}^{(2)} | \Phi_{H(2s)}(\rho) \rangle \quad (26)$$

In order to test the effect of polarization of H(2s), we switch on the polarization potentials of H(2s) atom, i.e.,

$V_{pol}^{H(2s)}(\sigma)$. This can be done by replacing $U_{st}^{(2)}(\sigma)$ by a potential $U^{(2)}(\sigma)$, such that

$$U^{(2)}(\sigma) = U_{st}^{(2)}(\sigma) + \lambda V_{pol}^{H(2s)}(\sigma) \quad (27)$$

The parameters λ appearing in Eq. (27) is introduced for distinguishing the various conditions (models) under which Eq. (23) and Eq. (24) are solved. Thus, we distinguish the following cases:

1. $\lambda=0$ (model I). This case is identical with the coupled static approximation, where no polarization effect is taken into account (we only considered the static potentials $U_{st}^{(1)}(x)$ and $U_{st}^{(2)}(\sigma)$).
2. $\lambda=1$. This case corresponds (model II) in which the polarization potential, $V_{pol}^{H(2s)}(\sigma)$, of channel 2 is added to $U_{st}^{(2)}(\sigma)$, while the coupled static picture of the system is considered. $V_{pol}^{H(2s)}(\sigma)$, which is added to include all p-states of $n=2$, i.e., H(2s+2p), is defined by (see ref. [14]):

We take

$$\Phi_{H(np)}(\rho) = \left(\frac{8}{43}\right)^{\frac{1}{2}} \rho \left(1 + \frac{\rho}{2}\right) e^{-\rho} \quad (28)$$

$$V(\sigma) = \langle \Phi_{H(2s)}(\rho) | V_{int}^{(2)} | \Phi_{H(np)}(\rho) \rangle \quad (29)$$

and

$$U(\sigma) = \langle \Phi_{H(np)}(\rho) | V_{int}^{(2)} | \Phi_{H(np)}(\rho) \rangle \quad (30)$$

Then,

$$V_{pol}^{H(2s)}(\sigma) = \beta(\sigma) V(\sigma) \quad (31)$$

where the function $\beta(\sigma)$ is calculated as follows: we take $\Delta E = E_{H(2s)} - E_{H^*}$, where $E_{H(2s)} = -0.25$ Ryd is the first excited 2s-state energy of H, $E_{H^*} = -21/129$ Ryd is the binding energy of the polarized hydrogen, and $w = \Delta E/V(\sigma)$. Also, we consider the two functions β^\pm such that $\beta^\pm(\sigma) = \frac{1}{2} \left\{ -w \pm (w^2 + 4)^{\frac{1}{2}} \right\}$.

The adiabatic energy of H(2s) within the field of a unit positive charge is found to be:

$$E_{ad}^{H(2s)} = \left\{ E_{H(2s)} + U_{st}^{(2)} + 2(\beta^\pm) V + [E_{H^*} + U](\beta^\pm)^2 \right\} / \left[1 + (\beta^\pm)^2 \right] \quad (32)$$

the correct β for calculating $V_{\text{pol}}^{\text{H}(2s)}(\sigma)$ is that one of β^+ and β^- which yields a minimum value for $E_{\text{ad}}^{\text{H}(2s)}$.

Using partial wave expansions of the scattering wave functions $|\psi_1\rangle$ and $|\psi_2\rangle$ in Eqs. (23) and (24), that solutions is given (formally) by the Lippmann-Schwinger equation:

$$|\xi\rangle = |\xi_0\rangle + G_0|\zeta\rangle \quad (33)$$

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

$$(\varepsilon - H_0)|\xi_0\rangle = |0\rangle \quad (34)$$

The partial wave expansions of Green operators corresponding to the operators in the two differential equations enable us to write their solutions in integral forms, that can be solved by iterative numerical technique. Then, we obtain the reactance matrix R^ν , that is related to the transition matrix T^ν by (see Appendix):

$$T^\nu = R^\nu (I - iR)^\nu \quad (35)$$

where ν is order of iteration, I is a 2×2 unit matrix, and $\tilde{i} = \sqrt{-1}$. The partial cross-sections obtained by the iterative way are determined (in πa_0^2 units) using the relation:

$$\sigma_{ij}^{(\ell, \nu)} = \frac{4(2\ell + 1)}{k_1^2} |T_{ij}^\nu|^2, \quad i = 1, 2 \quad (36)$$

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

$$\sigma_{ij}^\nu = \sum_{\ell=0}^{\infty} \sigma_{ij}^{(\ell, \nu)}, \quad i, j = 1, 2 \quad \nu > 0 \quad (37)$$

3 Results and Discussion

We start our investigation by testing the variation of the static potential of the first channel, $U_{\text{st}}^{(1)}(x)$, and the modified potential, $U^{(2)}(\sigma)$ of the second channel, with increase of x and σ , respectively. Values of x and σ have been chosen such that $x = \sigma = \frac{1}{16}, \frac{2}{16}, \frac{3}{16}, \dots, \frac{512}{16}$ where $h = \frac{1}{16}$ is the mesh size (or Simpson's step) employed for calculating integrals appearing in integral equations using Simpson's rule. Calculation of cross-sections of proton-sodium (p-Na) scattering has been proceeded by investigating variation of elements of R^ν with increase of integration range (IR) and the number of iterations. We have fixed h at $\frac{1}{16}$ and have obtained all the results presented below with

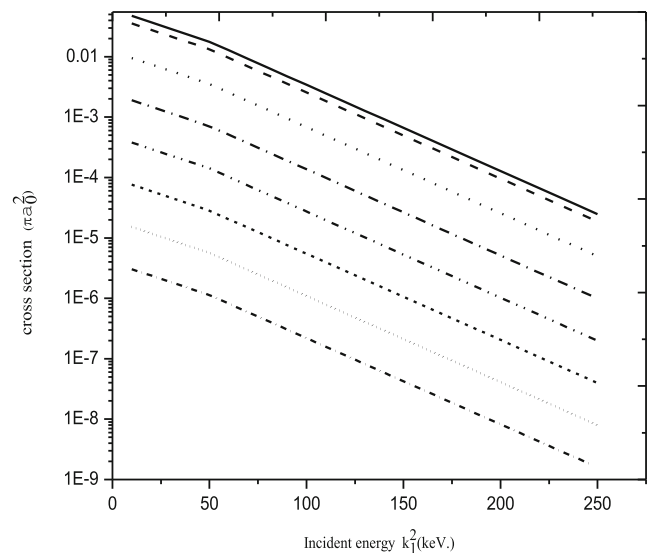


Fig. 2 Present partial and total elastic cross-sections (in πa_0^2) of p-Na scattering (model I) for the angular momentum ℓ : — $\ell=0$, \cdots $\ell=1$, — · — $\ell=2$, — · — · $\ell=3$, — · — · — $\ell=4$, $\ell=5$, — · — · — $\ell=6$, — total

512 mesh points (i.e., IR=32 a_0). It is found that excellent convergence can be obtained with $\nu=50$. This demonstrates the stability of our iterative method. Final calculations have been carried out for seven partial waves corresponding to $0 \leq \ell \leq 6$ at values of k_1^2 representing the kinetic energy region ($10 \leq k_1^2 \leq 1000$ keV).

To discuss the results of the present work for the partial and total cross-sections at the considered energies, Figs. 2, 3, 4, and 5 present the partial and total elastic and H(2s) formation cross-sections of models I and II at range of incident energy given by ($k_1^2 \leq 250$ keV) for seven values of the total angular

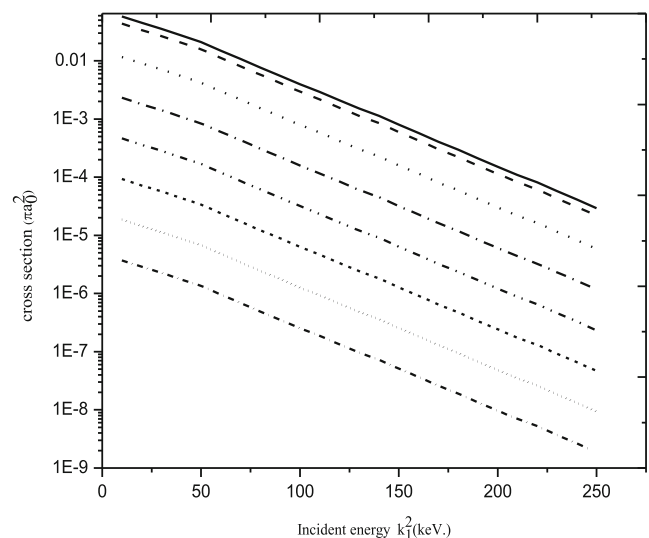


Fig. 3 Present partial and total elastic cross-sections (in πa_0^2) of p-Na scattering (model II) for the angular momentum ℓ : — $\ell=0$, \cdots $\ell=1$, — · — $\ell=2$, — · — · $\ell=3$, — · — · — $\ell=4$, $\ell=5$, — · — · — $\ell=6$, — total

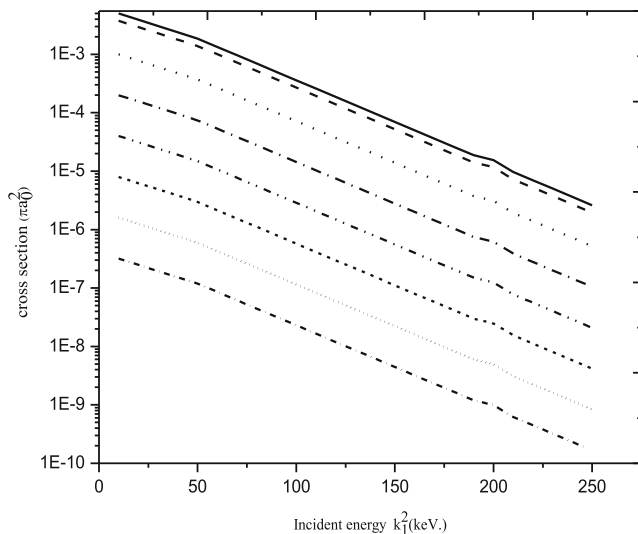


Fig. 4 Present partial and total H(2s) formation cross-sections (in πa_0^2) of p-Na scattering (model I) for the angular momentum ℓ : — $\ell=0$, \cdots $\ell=1$, — · — $\ell=2$, — · — · $\ell=3$, — — — $\ell=4$, \cdots $\ell=5$, — · — · $\ell=6$, — total

momentum ℓ ($0 \leq \ell \leq 6$). The figures indicate that the main contributions to the total elastic and H(2s) formation cross-sections of models I and II are due to the S and P partial cross-sections. The values of the cross sections for the two models decrease steadily with k_1^2 and the seven partial waves employed are quite satisfactory for calculating them. The seven partial waves employed are quite satisfactory for calculating the present values of the total cross-sections. The total elastic cross-sections σ_{11} of model II (inclusion of $V_{\text{pol}}^{H(2s)}(\sigma)$) are slightly larger than those of model I (neglecting polarization effect). The most interesting results are presented in Table 1 for the range of energy between 10 and 1000 keV.

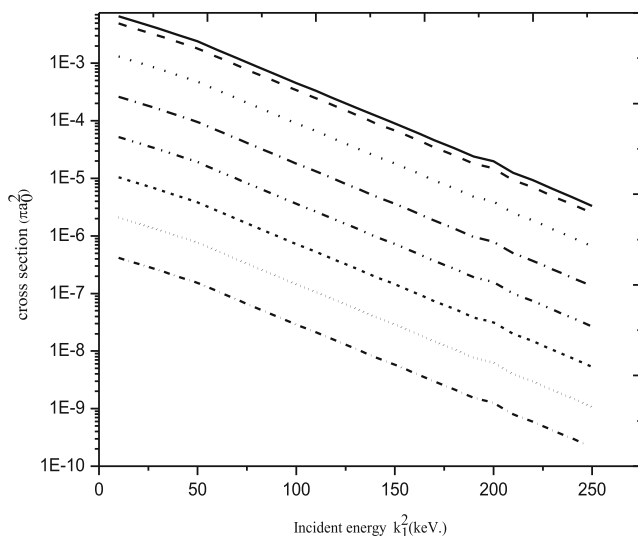


Fig. 5 Present partial and total H(2s) formation cross-sections (in πa_0^2) of p-Na scattering (model II) for the angular momentum ℓ : — $\ell=0$, \cdots $\ell=1$, — · — $\ell=2$, — · — · $\ell=3$, — — — $\ell=4$, \cdots $\ell=5$, — · — · $\ell=6$, — total

Table 1 Present total H(2s) cross sections formation (σ_{12} in πa_0^2) of p-Na scattering (two Models) with compared theoretical results ([7] and [8])

k_1^2 keV	σ_{12} Model I	σ_{12} Model II	σ_{12} [7]	σ_{12} [8]
10	4.9911E-03	6.5438E-03		
20	3.8993E-03	5.1124E-03		
30	3.0463E-03	4.0306E-03		
40	2.3799E-03	3.0967E-03		
50	1.8593E-03	2.4045E-03	1.16E-03	5.269E-03
60	1.3387E-03	1.7048E-03		
70	9.6385E-04	1.2263E-03		
80	6.9399E-04	8.7213E-04		
100	3.5976E-04	4.5126E-04	8.27E-05	4.912E-03
150	6.9611E-05	9.0718E-05	2.41E-05	1.827E-03
200	1.5509E-05	1.9798E-05	1.03E-05	5.206E-04
250	2.6062E-06	3.3269E-06		
300	1.7914E-06	2.3226E-06		
500	4.8091E-07	6.1669E-07	2.91E-07	6.022E-07
800	2.5552E-07	3.2618E-07		1.029E-07
1000	2.3988E-08	3.0735E-08		1.105E-08

and showed in Fig. 6 for the incident energy between 10 and 200 keV, where we find a comparison between total H(2s) formation cross-sections (in πa_0^2) determined by different authors using different approaches. In columns 2 and 3 of Table 1, we show the present total H(2s) formation cross-sections for the two models. Column 4 gives the values of H(2s) formation total cross-sections obtained by Choudhury and Sural [7] using the wave formulation of the impulse approximation to the case of electron capture into excited 2s state of hydrogen in collisions between protons and sodium atom. The next column contains total cross-sections of the formation of the H atom in the 2s excited state of proton–

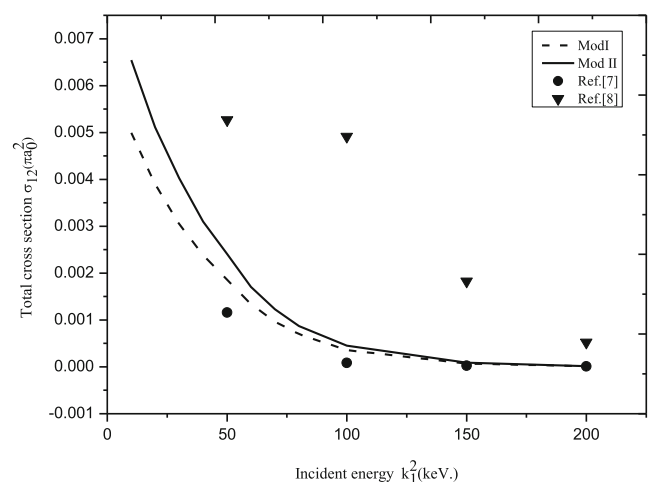


Fig. 6 Present total H(2s) formation cross-sections (σ_{12} in πa_0^2) of p-Na scattering (model II) with compared theoretical results ([7] and [8])

sodium scattering by using the Coulomb-projected Born (CPB) approximation given by Tiwari [8]. The present values of the total H(2s) cross-sections for the two models are in good agreement with those of Choudhury and Sural [7] for energies between 50 and 200 keV and lower than those of Tiwari [8] for $10 \leq k_1^2 \leq 150$ keV. Our total H(2s) cross-sections for the two models at 200 keV are in good agreement with those of Tiwari [8]. The reason for the difference lies in the different approximation used for the scattering wave function and in taking polarization potential of H(2s) in our calculations that are neglected in the compared results. Before leaving this section, it is important to mention that further improvements upon the present total collisional cross-sections can be also obtained by taking the excitation 2p-channel of hydrogen formation into account (which is now under consideration by the author). We notice that $V_{\text{pol}}^{\text{H}(2s)}(\sigma)$ has positive influence upon total cross-sections σ_{12} in the considered range of incident energy.

4 Conclusions

Proton–sodium inelastic scattering is studied using the coupled static approximation. Our interest is focused on the influence of the polarization potential of the H(2s) formation channel. The switching on $V_{\text{pol}}^{\text{H}(2s)}(\sigma)$ has positive influence upon total elastic and hydrogen (2s-state) formation cross-sections. The present calculations show reasonable agreement with available theoretical calculations in a wide range of energies.

Acknowledgments We are greatly indebted to Prof. M. A. Abdel-Raouf for his interest in this work and useful discussions.

Appendix

Our main goal in this appendix is to calculate the reactance matrix R.

Let us consider the partial wave expansions of the scattering wave functions $|\psi_1\rangle$ and $|\psi_2\rangle$, i.e.,

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

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

where $f_\ell(x)$ and $g_\ell(x)$ are the radial partial wave functions corresponding to the total angular momentum ℓ of the first and

second channels, respectively, $Y_\ell^0(\hat{x})$ and $Y_\ell^0(\hat{\sigma})$ are the related spherical harmonics, \hat{x} and $\hat{\sigma}$ are the angles between the vectors \vec{x} and $\vec{\sigma}$, and the z-axis.

Substitution from Eqs. (1) and (2) into Eqs. (23) and (24), we obtain for each value of ℓ , following the coupled integro-differential equations:

$$\left[\frac{d^2}{dx^2} - \frac{\ell(\ell+1)}{x^2} + k_1^2 \right] f_\ell(x) = 2\mu_M U_{\text{st}}^{(1)}(x) f_\ell(x) + \int_0^\infty K_{12}(x, \sigma) g_\ell(\sigma) d\sigma \quad (3)$$

And

$$\left[\frac{d^2}{d\sigma^2} - \frac{\ell(\ell+1)}{\sigma^2} + k_2^2 \right] g_\ell(\sigma) = 2\mu_{M'} U_{\text{st}}^{(2)}(\sigma) g_\ell(\sigma) + \int_0^\infty K_{21}(x, \sigma) f_\ell(x) dx \quad (4)$$

where the Kernels K_{12} and K_{21} are expanded by:

$$K_{12}(x, \sigma) = 2\mu_M (8\sigma x) \iint \Phi_{\text{Na}(3s)}(r) \Phi_{\text{H}(2s)}(\rho) \left[-\frac{1}{2\mu_{M'}} (\nabla_\sigma^2 + k_2^2) + V_{\text{int}}^{(2)} \right] Y_\ell^0(\hat{x}) Y_\ell^0(\hat{\sigma}) d\hat{x} d\hat{\sigma} \quad (5)$$

and

$$K_{21}(x, \sigma) = 2\mu_{M'} (8\sigma x) \iint \Phi_{\text{Na}(3s)}(r) \Phi_{\text{H}(2s)}(\rho) \left[-\frac{1}{2\mu_M} (\nabla_x^2 + k_1^2) + V_{\text{int}}^{(1)} \right] Y_\ell^0(\hat{x}) Y_\ell^0(\hat{\sigma}) d\hat{x} d\hat{\sigma} \quad (6)$$

The number 8 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. (3) and (4) as:

$$\left[\frac{d^2}{dx^2} - \frac{\ell(\ell+1)}{x^2} + k_1^2 \right] f_\ell(x) = 2\mu_M U_{\text{st}}^{(1)}(x) f_\ell(x) + Q_1(x) \quad (7)$$

and

$$\left[\frac{d^2}{d\sigma^2} - \frac{\ell(\ell+1)}{\sigma^2} + k_2^2 \right] g_\ell(\sigma) = 2\mu_{M'} U_{\text{st}}^{(2)}(\sigma) g_\ell(\sigma) + Q_2(\sigma) \quad (8)$$

where

$$Q_1(x) = \int_0^\infty K_{12}(x, \sigma) g_\ell(\sigma) d\sigma \quad (9)$$

and

$$Q_2(\sigma) = \int_0^\infty K_{21}(x, \sigma) f_\ell(x) dx \quad (10)$$

The solutions of Eqs.(7) and (8) are given formally (using Lippmann-Schwinger equation) by:

$$f_\ell^{(i)}(x) = \left\{ \delta_{i1} + \frac{1}{k_1} \int_0^\infty \tilde{g}_\ell(k_1 x') \left[2\mu_M U_{st}^{(1)}(x') f_\ell^{(i)}(x') + Q_1^{(i)}(x') \right] dx' \right\} \tilde{f}_\ell(k_1 x) \\ + \left\{ -\frac{1}{k_1} \int_0^\infty \tilde{f}_\ell(k_1 x') \left[2\mu_M U_{st}^{(1)}(x') f_\ell^{(i)}(x') + Q_1^{(i)}(x') \right] dx' \right\} \tilde{g}_\ell(k_1 x) \quad i=1, 2 \quad (11)$$

and

$$g_\ell^{(i)}(\sigma) = \left\{ \delta_{i1} + \frac{1}{k_2} \int_0^\infty \tilde{g}_\ell(k_2 \sigma') \left[2\mu_M U_{st}^{(2)}(\sigma') g_\ell^{(i)}(\sigma') + Q_2^{(i)}(\sigma') \right] d\sigma' \right\} \tilde{f}_\ell(k_2 \sigma) \\ + \left\{ -\frac{1}{k_2} \int_0^\infty \tilde{f}_\ell(k_2 \sigma') \left[2\mu_M U_{st}^{(2)}(\sigma') g_\ell^{(i)}(\sigma') + Q_2^{(i)}(\sigma') \right] d\sigma' \right\} \tilde{g}_\ell(k_2 \sigma) \quad i=1, 2 \quad (12)$$

where the delta functions δ_{ij} , $i, j=1, 2$, specify two independent forms of solutions for each of $f_\ell(x)$ and $g_\ell(x)$ in channels $i=1$ and 2, 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 $i=2$, this element will be 0, defining the second form. The functions $\tilde{f}_\ell(\mu)$ and $\tilde{g}_\ell(\mu)$ and $\mu=k_1 x$ or $k_2 \sigma$ are related to the Bessel functions of the first and second channels, i.e., $j_\ell(\mu)$ and $y_\ell(\mu)$, respectively, by the relations $\tilde{f}_\ell(\mu) = \mu j_\ell(\mu)$ and $\tilde{g}_\ell(\mu) = -\mu y_\ell(\mu)$.

It is obvious from Eqs. (11) and (12) that the solutions can be only found iteratively and the ν th iteration are calculated by :

$$f_\ell^{(i, \nu)}(x) = \left\{ \delta_{i1} + \frac{1}{k_1} \int_0^x \tilde{g}_\ell(k_1 x') \left[2\mu_M U_{st}^{(1)}(x') f_\ell^{(i, \nu)}(x') + Q_1^{(i, \nu-1)}(x') \right] dx' \right\} \tilde{f}_\ell(k_1 x) \\ + \left\{ -\frac{1}{k_1} \int_0^x \tilde{f}_\ell(k_1 x') \left[2\mu_M U_{st}^{(1)}(x') f_\ell^{(i, \nu)}(x') + Q_1^{(i, \nu-1)}(x') \right] dx' \right\} \tilde{g}_\ell(k_1 x) \\ i=1, 2; \quad \nu \geq 1 \quad (13)$$

and

$$g_\ell^{(i, \nu)}(\sigma) = \left\{ \delta_{i1} + \frac{1}{k_2} \int_0^\infty \tilde{g}_\ell(k_2 \sigma') \left[2\mu_M U_{st}^{(2)}(\sigma') g_\ell^{(i, \nu)}(\sigma') + Q_2^{(i, \nu)}(\sigma') \right] d\sigma' \right\} \tilde{f}_\ell(k_2 \sigma) \\ + \left\{ -\frac{1}{k_2} \int_0^\infty \tilde{f}_\ell(k_2 \sigma') \left[2\mu_M U_{st}^{(2)}(\sigma') g_\ell^{(i, \nu)}(\sigma') + Q_2^{(i, \nu)}(\sigma') \right] d\sigma' \right\} \tilde{g}_\ell(k_2 \sigma) \\ i=1, 2; \quad \nu \geq 1 \quad (14)$$

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

$$f_\ell^{(i, 0)}(x) = \left\{ \delta_{i1} + \frac{1}{k_1} \int_0^x \tilde{g}_\ell(k_1 x') \left[2\mu_M U_{st}^{(1)}(x') f_\ell^{(i, 0)}(x') \right] dx' \right\} \tilde{f}_\ell(k_1 x) \\ + \left\{ -\frac{1}{k_1} \int_0^x \tilde{f}_\ell(k_1 x') \left[2\mu_M U_{st}^{(1)}(x') f_\ell^{(i, 0)}(x') \right] dx' \right\} \tilde{g}_\ell(k_1 x) \\ i=1, 2 \quad (15)$$

where X and Σ specify the integration range (IR) away from the nucleus over which the integrals at Eqs.(13)–(15) are calculated using Simpson's expansions. The functions $Q_1^{(i, \nu-1)}(x')$ and $Q_2^{(i, \nu)}(\sigma')$, in Eqs.(13) and (14), are now defined by:

$$Q_1^{(i, \nu-1)}(x') = \int_0^\Sigma K_{12}(x', \sigma) g_\ell^{(i, \nu-1)}(\sigma') d\sigma', \quad \nu \geq 1 \quad (16)$$

$$Q_2^{(i, \nu)}(\sigma') = \int_0^X K_{21}(x, \sigma') f_\ell^{(i, \nu)}(x) dx, \quad \nu \geq 0 \quad (17)$$

Thus, the iteration process starts by calculating by $f_\ell^{(i, \nu)}(x)$, $i=1, 2$ using Eq. (13) and introducing its values into Eq. (17) in order to find $Q_2^{(i, 0)}(\sigma')$ which can be used in the right-hand side of Eq. (14) for obtaining $g_\ell^{(i, 0)}(\sigma)$. The values of the last quantity can be introduced into Eq. (17) in order to calculate $Q_1^{(i, 0)}(x')$ which may be employed in Eq.(13) for determining $Q_2^{(i, 1)}(x)$. 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}^ν where ν increase (note that $f_\ell^{(i, \nu)}(0)=g_\ell^{(i, \nu)}(0)=0$). In order to find the starting value of $f_\ell^{(i, 0)}(x)$, we consider the Taylor expansion of $U_{st}^{(1)}(x)$, $\tilde{f}_\ell(k_1 x)$ and $\tilde{g}_\ell(k_1 x)$ around the origin. For further information about the numerical techniques employed in this paper, see ref. [14].

Eqs. (13) and (14) can be abbreviated to:

$$f_{\ell}^{(i,v)}(x) = a_1^{(i,v)} \tilde{f}_{\ell}(k_1 x) + b_1^{(i,v)} \tilde{g}_{\ell}(k_1 x), \quad i = 1, 2 \quad (18)$$

$$g_{\ell}^{(i,v)}(\sigma) = a_2^{(i,v)} \tilde{f}_l(k_2 \sigma) + b_2^{(i,v)} \tilde{g}_l(k_2 \sigma), \quad i = 1, 2 \quad (19)$$

where

$$a_1^{(i,v)} = \{\}_1, b_1^{(i,v)} = \{\}_2, a_2^{(i,v)} = \{\}_3, b_2^{(i,v)} = \{\}_4$$

The coefficients at Eqs. (16) and (17) are elements of the following matrices:

$$a^v = \begin{pmatrix} \sqrt{2\mu_M/k_1} a_1^{(1,v)} & \sqrt{2\mu_M/k_1} a_1^{(2,v)} \\ \sqrt{2\mu_{M'}/k_2} a_2^{(1,v)} & \sqrt{2\mu_{M'}/k_2} a_2^{(2,v)} \end{pmatrix} \quad \text{and} \quad (20)$$

$$b^v = \begin{pmatrix} \sqrt{2\mu_M/k_1} b_1^{(1,v)} & \sqrt{2\mu_M/k_1} b_1^{(2,v)} \\ \sqrt{2\mu_{M'}/k_2} b_2^{(1,v)} & \sqrt{2\mu_{M'}/k_2} b_2^{(2,v)} \end{pmatrix}$$

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

$$R^v = b^v (a^v)^{-1}. \quad (21)$$

References

1. M.A. Abdel-Raouf, S.A. Elkilany, Int. J. Pure and Appl. Phys. **5**(2), 93 (2009)
2. K. E Banyard, G. W. Shirtcliffe, J. Phys. B: atom. Mol. Phys. **12**(19), 3247 (1979)
3. G. Ferrante, E. Fiordilino, M. Zarcone, IL Nuovo Cimento **52B**(2), 151 (1979)
4. R. Daniele, G. Ferrante, E. Fiordilino, IL Nuovo Cimento **54B**(1), 185 (1979)
5. G. Ferrante, E. Fiordilino, IL Nuovo Cimento **57B**, 1 (1980)
6. W. Fritsch, C.D. Lin, J. Phys. B: at. Mol. Phys. **16**, 1595 (1983)
7. K.B. Choudhury, D.P. Sural, J. Phys. B: at. Mol. Phys. **25**, 853 (1992)
8. Y.N. Tiwari, Pramana-journal of physics **70**(4), 753 (2008)
9. S. A. Elkilany, M. A. Abdel-Raouf, Journal Phys B 388, Article ID 072030 (2012)
10. S.A. Elkilany, Indian. J. Phys. **88**(1), 19 (2014)
11. S.A. Elkilany, J. Theor. Chem. **2014**, 1 (2014)
12. M A Abdel-Raouf J. Phys. B: At. Mol. Opt. Phys. **21** 2331 (1988)
13. E. Clementi, C. Roetti, Atomic Data Nuclear Data Tables **14**(3–4), 177 (1974)
14. M.A. Abdel-Raouf, Acta Phys. Hung. **63**(1–2), 21–50 (1988)