Electron capture in ground and excited states in proton–alkali-metal-atom collisions

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Abstract. The wave formulation of the impulse approximation has been applied 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 caesium. 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. Wherever possible our results have been compared with other available results.

1. Introduction

Beams of high energy neutral particles which are used in prototype fusion reactors for plasma heating and fuelling are efficiently produced by neutralization of accelerated positive ions while passing through a metallic vapour target such as that containing alkali-metal atoms (Gilbody 1979, Ferrante and Fiordilino 1980). A typical process of the type

$$H^+ + X \rightarrow X^+ + H(n, l, m) \tag{1}$$

where X is an alkali metal atom, is capable of producing intense energetic neutral beams. Up to now several theoretical methods have been developed (Basu *et al* 1978, Janev *et al* 1985, Bransden and Dewangan 1989, Crothers and Dunseath 1987, 1990) to study the process of electron capture in ion–atom collisions but in most cases applications have been made to capture from light atoms like hydrogen and helium. Electron capture by high energy protons from alkali-metal atoms have not been studied extensively. Theoretically this study is complicated due to the many-electron character of the target alkali-metal atom. However for many practical purposes the alkali-metal atoms may be considered as one-electron systems with some model potentials. In particular if one considers only valence electron capture, one can treat the alkali-metal atom as a one-electron model atom (Bardsley 1974) where the loosely bound valence electron is supposed to be acted upon by a model potential taking into account the joint effect of the nucleus and the core electrons.

In the present work we have investigated the charge transfer process (1), where we have considered charge transfer into the ground and excited 2s and 2p states of the hydrogen atom. X and X^+ represent the ground states of any of the alkali-metal atoms

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from sodium to caesium and the corresponding ion, respectively. We have used the wave formulation of the impulse approximation (Pradhan 1957, Coleman and McDowell 1965) which is a second-order method allowing for the continuum intermediate states, and is applicable if the effective duration of the collision is small compared to the orbital period of the bound electron. This method is an improvement over the first-order methods from the point of view of the physics involved. Different workers have studied many variations of this approximation (see, for example, Briggs 1977, Belkic *et al* 1979). Recently Taulbjerg *et al* (1990) have formulated the strong potential Born (SPB) approximation including the effects of elastic scattering in the initial and final channels. They have found that the channel modified SPB wavefunction has the impulse approximation as a limiting form when a suitable channel potential is used. The present method gives us directly the differential cross sections for the process and the integral cross sections can then be obtained by integration over the scattering angle. This approximation is essentially a high energy approximation and so far no work has been performed on the capture into excited states of hydrogen in proton–alkali-atom collisions in the high energy limit. However, in recent years some attention has been focused on the theoretical and experimental study of this process in the low energy region (Kimura *et al* 1982, Fritsch 1984, Dowek *et al* 1990, Ebel and Salzborn 1983) where it is found that the cross section for capture in the $n = 2$ state is greater than that in the ground state.

During the study of the capture into the excited states of hydrogen we have also obtained the results for capture into the ground state of hydrogen. In another approach, Daniele *et al* (1979) have used an eikonal approximation treatment to obtain the integral cross sections for the ground-state capture for the high energy proton–alkalimetal-atom charge transfer problem.

We explain the theory of the method used by us in section 2. The evaluation of the integrals occurring in the transition matrix elements and the numerical techniques used are explained in the appendix and section 2.1, respectively. The differential and integral cross sections for electron capture into the ground and 2s, 2p excited states are presented and discussed in section 3.

Atomic units will be used throughout except for the integral cross sections, which will be expressed in πa_0^2. The differential cross sections are expressed in the laboratory frame which are obtained from the centre-of-mass frame by the usual transformation.

2. Theory

We shall denote the incident proton (particle 3) as the particle A^+ of charge Z_A and mass M_A. The valence electron e^- being captured will be called particle 1 and Z_B, M_B will represent, respectively, the initial charge and mass of the alkali-metal core which will be denoted by $B^+(2)$. In the initial state (denoted by i), the particle 1 is bound to the ion B^+ and in the final state (denoted by f), the particle 1 is bound to particle 3. r_{1B} and r_{1A} locate the electron with respect to the ions B^+ and A^+, respectively. R_i is the position vector of the ion A^+ relative to the centre of mass of the atom B, R_f is the position vector of the centre of mass of the atom A relative to the ion B^+ and k_i, k_f are the initial and final relative momenta, respectively. R is the separation vector from B^+ to A^+. The post form of the impulse approximation transition matrix element for the process (1) can be written as

$$T_{if} = \langle \psi_r^f | V_r | \Psi_i^{\text{imp}} \rangle \tag{2}$$

where $|\psi_r^f\rangle$ represents the unperturbed state in the final channel, $V_r = V_{AB} + V_{Be}$ is the post interaction, and

$$|\Psi_i^{Imp}\rangle = (1 + b_{Ae}^+ + b_{AB}^+)|\psi_d^i\rangle. \tag{3}$$

Here $|\psi_d^i\rangle$ denotes the unperturbed state in the initial channel and the operator b_{ij}^+ is

$$b_{ij}^+ = \int \frac{1}{E_m - H_0 - V_{ij} + i\varepsilon} \, V_{ij}|\chi_m\rangle \, dm\langle\chi_m| \tag{4}$$

where H_0 is the total kinetic energy operator, V_{ij} is the interaction between the particles i and j, $|\chi_m\rangle$ represents the eigenvector of the total kinetic energy operator with eigenvalue E_m and ε is the usual infinitesimal positive quantity. In writing (2) the multiple scattering terms are neglected (Coleman 1969). These will be zero if the interaction between A^+ and B^+ is omitted and, for heavy particle collisions, it is the standard practice to omit V_{AB} throughout and put b_{AB}^+ in (3) equal to zero. Any error due to the omission of V_{AB} is expected to be small and decreases with increasing incident energy. It may be noted that we have used the post form of the transition matrix element. One can of course use the prior form as well but, in an earlier work on electron capture by protons from alkali-metal-like ions using the Coulomb Born approximation and similar types of model potentials, Sinha *et al* (1982) found their 'post' results to be in better agreement with experimental observations than the 'prior' ones. In view of the heavy computational effort required for the calculation using the impulse approximation, we have worked with only the post form of the transition matrix element.

The unperturbed states in the initial and final channel can be expressed in coordinate representation as

$$\psi_d^i = \exp(i\mathbf{k}_i \cdot \mathbf{R}_i)\varphi_{Bi}(\mathbf{r}_{1B}) \qquad \psi_r^f = \exp(i\mathbf{k}_f \cdot \mathbf{R}_f)\varphi_{Af}(\mathbf{r}_{1A}) \tag{5}$$

where φ_{Af} is the final-state wavefunction of the hydrogen atom formed by electron capture and φ_{Bi} is the wavefunction of the ground state of the alkali atom.

After some analytical work following a procedure similar to Coleman (1969), the impulse approximation wavefunction reduces to

$$\Psi_i^{Imp}(\mathbf{R}_f, \mathbf{r}_{1A}) = (2\pi a)^{-3} \int d\mathbf{q}\, N(\nu_q) g_i\left(-\mathbf{v} - \frac{1}{a}\mathbf{q}\right) {}_1F_1(-i\nu_q; 1; i(qr_{1A} - \mathbf{q} \cdot \mathbf{r}_{1A}))$$

$$\times \exp\{i(\mathbf{k}_i/a + \mathbf{q}/a) \cdot \mathbf{R}_f\} \exp(i\mathbf{q} \cdot \mathbf{r}_{1A}) \tag{6}$$

where

$$a = M_A/(M_A + 1) \qquad \nu_q = -Z_A/(q/a) \qquad N(\nu_q) = \exp(-\tfrac{1}{2}\pi\nu_q)\Gamma(1 + i\nu_q)$$

$$g_i(\mathbf{t}_1) = \int \varphi_{Bi}(\mathbf{r}_{1B}) \exp(i\mathbf{t}_1 \cdot \mathbf{r}_{1B}) \, d\mathbf{r}_{1B}$$

and $\mathbf{v}$ is the relative velocity in the incident channel and, consequently, from (2), the transition matrix element becomes,

$$T_{if} = (2\pi a)^{-3} \int\int\int \varphi_{Af}^*(\mathbf{r}_{1A}) \exp\{i(\mathbf{k}_i/a - \mathbf{k}_f + \mathbf{q}/a) \cdot \mathbf{R}_f + i\mathbf{q} \cdot \mathbf{r}_{1A}\}$$

$$\times V_{Be} N(\nu_q) g_i(-\mathbf{q}/a - \mathbf{v})$$

$$\times {}_1F_1(-i\nu_q; 1; i(qr_{1A} - \mathbf{q} \cdot \mathbf{r}_{1A})) \, d\mathbf{r}_{1A} \, d\mathbf{R}_f \, d\mathbf{q}. \tag{7}$$

The wavefunction $\varphi_{Bi}(r_{1B})$ for the ground state of any of the alkali-metal atoms from sodium to caesium is taken to be that given by Hart and Goodfriend (1970),

$$\varphi_{Bi}(r_{1B}) = D \exp(-\lambda_1 r_{1B}). \tag{8a}$$

The corresponding alkali-metal core-electron potential V_{Bc} is given by

$$V_{Bc} = -\frac{1}{r_{1B}} + \frac{A}{r_{1B}} \exp(-\lambda r_{1B}). \tag{8b}$$

The values of parameters D, λ_1, A and λ are taken from Hart and Goodfriend (1970) and reproduced in table 1 for convenience. φ_{Af} is the wavefunction of the 1s, 2s or 2p state of the hydrogen atom as the case may be.

Table 1. The parameters for the wavefunctions (8a) and core electron potentials (8b) of the alkali-metal atoms together with the binding energies (Hart and Goodfriend 1970). All quantities are in atomic units except the binding energies which are in eV.

	D	λ_1	A	λ	Binding energy (eV)
Sodium	0.113 6	0.3436	2.685	1.446	5.138
Potassium	0.094 47	0.3038	1.813	0.8320	4.341
Rubidium	0.093 82	0.3024	1.494	0.6606	4.176
Caesium	0.087 52	0.2887	1.371	0.5492	3.893

Substituting (8b) into (7) and using Fourier transforms we can write, on working out the integral over R_f,

$$T_{if} = -\frac{1}{2a\pi^2} \int\!\!\int \varphi_{Af}^*(r_{1A}) \exp(it \cdot r_{1A}) \left(\frac{1}{(q-t)^2} - \frac{A}{(q-t)^2 + \lambda^2 a^2} \right) N(\nu_q)$$

$$\times {}_1F_1(-i\nu_q; 1; i(qr_{1A} - q \cdot r_{1A})) g_i(-v - q/a) \, dr_{1A} \, dq \tag{9}$$

where

$$t = ak_f - k_i. \tag{10}$$

Substituting (8a) in the expression for $g_i(t_1)$ we obtain

$$g_i(t_1) = D \int \exp(it_1 \cdot r_{1B}) \exp(-\lambda_1 r_{1B}) \, dr_{1B} = 8\pi \frac{D\lambda_1}{(t_1^2 + \lambda_1^2)^2}. \tag{11}$$

Therefore,

$$T_{if} = -\frac{4D\lambda_1}{a\pi} \int\!\!\int \varphi_{Af}^*(r_{1A}) \exp(it \cdot r_{1A}) N(\nu_q) {}_1F_1(-i\nu_q; 1; i(qr_{1A} - q \cdot r_{1A}))$$

$$\times \left(\frac{1}{(q-t)^2} - \frac{A}{(q-t)^2 + \lambda^2 a^2} \right) \frac{1}{[(v+q/a)^2 + \lambda_1^2]^2} \, dr_{1A} \, dq \tag{12a}$$

$$= -\frac{4D\lambda_1 a^3}{\pi} \int F_f(q, t) \left(\frac{1}{(t-q)^2} - \frac{A}{(t-q)^2 + \lambda^2 a^2} \right) N(\nu_q) P_1(q) \, dq \tag{12b}$$

where $F_f(q, t)$ is given by

$$F_f(q, t) = \int \varphi^*_{Af}(r_{1A}) \exp(it \cdot r_{1A}) {}_1F_1(-i\nu_q; 1; i(qr_{1A} - q \cdot r_{1A})) \, dr_{1A} \tag{13}$$

and

$$P_1(q) = \frac{1}{[(av + q)^2 + \lambda_1^2 a^2]^2}. \tag{14}$$

Depending on whether the final state f is the 1s, 2s or 2p state of the hydrogen atom, we have different expressions for the function F_f. The methods of evaluation of the integrals are explained in the appendix. The transition matrix element for capture into the ground state of hydrogen is

$$T_{i1s} = -\frac{32(aZ_A)^{3/2}a^3 D\lambda_1}{\pi^{1/2}} \int N(\nu_q) \left(\frac{(1 + i\nu_q)aZ_A}{T^2} + \frac{(-i\nu_q)(aZ_A - iq)}{T[T - 2(iaZ_A q + t \cdot q)]} \right)$$

$$\times P_2(q) \left(\frac{1}{(q - t)^2} - \frac{A}{(q - t)^2 + \lambda^2 a^2} \right) P_1(q) \, dq \tag{15}$$

where

$$P_2(q) = \left(\frac{T}{T - 2(iaZ_A q + t \cdot q)} \right)^{-i\nu_q} \qquad T = a^2 Z_A^2 + t^2. \tag{16}$$

After transforming the functions $P_1(q)$ and $P_2(q)$ to forms suitable for numerical computation, the integrals (15) for different energies and scattering angles are evaluated numerically using the techniques described in section 2.1. The expression for T_{i2s}, the transition matrix element for the 2s-state capture process, and those for T_{i2p_x}, T_{i2p_y} and T_{i2p_z}, the transition matrix elements for capture into the different substates of the 2p state are given in (A5) and (A9), respectively, of the appendix (with our choice of the axes T_{i2p_y} turns out to be zero). These are also computed for different energies and scattering angles following a procedure similar to that used for T_{i1s} and described below.

2.1. Numerical methods

The numerical integrations are performed on a Burroughs B6700 computer. A particular value of the scattering angle θ is first chosen for each value of the incident energy. The integration over ν (the polar angle of q as explained in the appendix) for a particular value of q is done separately in a subroutine using a Gaussian quadrature formula and this is repeated for all values of q. After checking for convergence, in most cases a 32-point quadrature formula is used. The integrals come out to be accurate up to ten significant figures in most cases and up to eight significant figures in the rest. The q integration has been performed by means of Simpson's integration technique. The range of integration was divided into three parts and separate small step sizes are chosen for each part. Convergence checks by using smaller step sizes and also by increasing the upper limit of q are done so that the final results of this integration are accurate up to six significant figures. The entire process is repeated for different values of θ for each incident energy and target atom.

The differential cross sections for electron transfer from an alkali-metal atom to the 1s, 2s and 2p states of the hydrogen atom are then given by

$$I^{1s(2s)}(\theta) = \frac{\mu_i \mu_f}{4\pi^2} \frac{k_f}{k_i} |T_{i1s(2s)}|^2 \qquad (17)$$

and

$$I^{2p}(\theta) = \frac{\mu_i \mu_f}{4\pi^2} \frac{k_f}{k_i} [|T_{i2p_x}|^2 + |T_{i2p_z}|^2] \qquad (18)$$

where μ_i and μ_f are the reduced masses in the initial and final channel respectively. k_f is obtained from the energy conservation equation. The cross sections in the laboratory system are obtained using the usual transformations.

The integral cross sections are obtained numerically from the relation

$$Q^{1s(2s,2p)} = 2\pi \int_0^\pi I^{1s(2s,2p)}(\theta) \sin\theta \, d\theta. \qquad (19)$$

The accuracy of the integral cross sections is estimated to be about three to four significant digits.

3. Results and discussions

The impulse approximation cross sections for electron capture into the ground, 2s and 2p states of hydrogen in proton–alkali-metal-atom collisions have been calculated for incident ion energy varying between 50 and 500 keV. The alkali-metal atoms chosen are sodium, potassium, rubidium and caesium. Table 2 shows the integral cross sections for charge transfer into the ground state of hydrogen for different incident energy values. The present results are depicted in the third column of this table. For completeness we present the results for sodium from the work of Basu Choudhury and Sural (1983). The results obtained using an eikonal approximation by Daniele *et al* (1979), who have used the same wavefunction and model parameters used by us, are presented in the fourth column of this table. Some estimated cross sections quoted by Daniele *et al* in the first Born approximation (FBA) have been presented in the last column of the table. These authors obtained these results by multiplying the Oppenheimer–Brinkman–Kramers (OBK) cross sections by the factor 0.66. It should be noted here that this scaling factor should actually vary with energy. At the lower end of the energy region, our results have the lowest value, followed by the eikonal results, the FBA cross sections having values even higher than these. However, in the higher energy region the FBA results lie much closer to our impulse approximation values than the eikonal cross sections. The reason for the difference between the cross sections obtained by our impulse approximation method and those obtained by Daniele *et al* (1979) lies in the different approximations used for the scattering wavefunction. In the impulse approximation, the scattering wavefunction contains the complete Coulomb wave arising out of the interaction between the incident ion and the electron. In the eikonal approximation, however, only the asymptotic part of this wave is retained.

Table 3 depicts the integral cross sections for charge transfer into the 2s state of hydrogen for the incident energy values varying between 50 and 500 keV for different alkali-metal atoms as target. It is found that, for all the alkali-metal atoms considered, the integral cross sections decrease as the energy increases from 50 to 500 keV. However,

Table 2. Integral cross sections for ground state electron capture in proton-alkali-metal atom collisions in units of πa_0^2. Present: impulse approximation results obtained in the present work (the results of sodium are taken from the work of Basu Choudhury and Sural (1983)). Eikonal: eikonal approximation results of Daniele *et al* (1979). FBA: estimated first Born approximation results quoted by Daniele *et al* (1979). (The bracketed numbers denote the powers of ten by which each entry should be multiplied.)

Target element	Incident energy (keV)	Present	Eikonal	FBA
Sodium	50	0.528 (−2)	0.135 (−1)[a]	0.933 (−1)[a]
	100	0.100 (−2)	0.398 (−2)	0.777 (−2)
	150	0.335 (−3)	0.132 (−2)[b]	0.454 (−3)[b]
	200	0.134 (−3)	0.421 (−3)	0.111 (−3)
	500	0.356 (−5)	—	—
Potassium	50	0.291 (−2)	0.334 (−2)[a]	0.426 (−1)[a]
	100	0.551 (−3)	0.109 (−2)	0.231 (−2)
	150	0.152 (−3)	0.405 (−3)[b]	0.140 (−3)[b]
	200	0.530 (−4)	—	—
	500	0.955 (−6)	—	—
Rubidium	50	0.115 (−2)	0.106 (−2)[c]	0.149 (−1)[c]
	100	0.214 (−3)	0.444 (−3)	0.239 (−2)
	150	0.604 (−4)	0.114 (−3)	0.478 (−4)
	200	0.210 (−4)	0.469 (−4)	0.197 (−4)
	500	0.369 (−6)	—	—
Caesium	50	0.741 (−3)	0.582 (−3)[c]	0.108 (−1)[c]
	100	0.134 (−3)	0.237 (−3)	0.163 (−2)
	150	0.359 (−4)	0.726 (−4)[b]	0.383 (−4)
	200	0.121 (−4)	0.247 (−4)	0.113 (−4)
	500	0.197 (−6)	—	—

[a] At 70 keV.
[b] At 140 keV.
[c] At 80 keV.

Table 3. Integral cross sections for 2s state electron capture in proton-alkali-metal-atom collisions in units of $10^{-2} \pi a_0^2$. (The bracketed numbers denote the powers of ten by which each entry should be multiplied.)

Incident proton energy (keV)	Integral cross sections ($10^{-2} \pi a_0^2$)			
	Sodium	Potassium	Rubidium	Caesium
50	0.116 (0)	0.638 (−1)	0.440 (−1)	0.311 (−1)
100	0.827 (−2)	0.434 (−2)	0.208 (−2)	0.134 (−2)
150	0.241 (−2)	0.106 (−2)	0.467 (−3)	0.282 (−3)
200	0.103 (−2)	0.368 (−3)	0.156 (−3)	0.913 (−4)
500	0.291 (−4)	0.805 (−5)	0.322 (−5)	0.174 (−5)

the general trend is that the rate of decrease of the cross section diminishes with increasing incident energy. Again, the rate of decrease for a particular energy range is found in general to increase as the atomic number of the target element is increased. It is also observed that the integral cross section for 2s capture for a particular value of incident proton energy decreases with increasing atomic number of the alkali-metal atoms. This is because of the type of wavefunction (8a) and model potential (8b) used, whose parameters are listed in table 1. The contribution of the second term of the model potential partly cancels that of the first term and the cancellation increases in going from sodium to caesium. Further, the parameter D of the wavefunction of the target atom, which remains a multiplying factor in the scattering amplitude decreases as the atomic number of the alkali-metal atom increases.

In table 4 we present the integral cross sections for charge transfer into the 2p state of hydrogen for the same energy range as considered in the case of 1s or 2s state capture for the different alkali-metal atoms. The variations of the cross sections with energy and target atomic number show the same types of trends as discussed in the previous paragraph for the 2s state capture. It is also found that the cross sections for electron capture into the $n = 2$ states are lower than the ground-state capture cross sections. However, the 2p state capture cross sections are smaller than the corresponding 2s state results. As there are no other theoretical or experimental results available at present for excited state capture in proton–alkali-metal-atom collisions in the high energy region, it is not possible to compare our data. However, in the case of $H^+ + H(1s) \rightarrow H(2s, 2p) + H^+$ reactions, the results obtained by Coleman and McDowell (1965) and by Coleman and Trelease (1968) also show that the 2s state capture cross sections are greater than the 2p state capture cross sections.

Table 4. Integral cross sections for 2p state capture in proton-alkali-metal-atom collisions in units of $10^{-2} \pi a_0^2$. (The bracketed numbers denote the powers of ten by which each entry should be multiplied.)

Incident proton energy (keV)	Integral cross sections ($10^{-2} \pi a_0^2$)			
	Sodium	Potassium	Rubidium	Caesium
50	0.770 (−1)	0.373 (−1)	0.215 (−1)	0.141 (−1)
100	0.683 (−2)	0.319 (−2)	0.137 (−2)	0.836 (−3)
150	0.170 (−2)	0.652 (−3)	0.269 (−3)	0.157 (−3)
200	0.515 (−3)	0.187 (−3)	0.758 (−4)	0.429 (−4)
500	0.840 (−5)	0.206 (−5)	0.803 (−6)	0.428 (−6)

Figures 1–3 show the differential cross sections for the ground state capture of a valency electron at incident energies 100, 200 and 500 keV in the case of proton–potassium, proton–rubidium and proton–caesium collisions. The differential cross sections at all energies become very small when the scattering angle exceeds a few mrad. As expected, a high peaking in the forward direction is observed, particularly in the higher energy end of the region studied. A distinct characteristic change in the slopes of the curves at small scattering angle is observed at 500 keV. It is interesting to note that the nature of the differential cross sections depends sensitively on the model potentials and wavefunctions used for the alkali atoms and consequently an
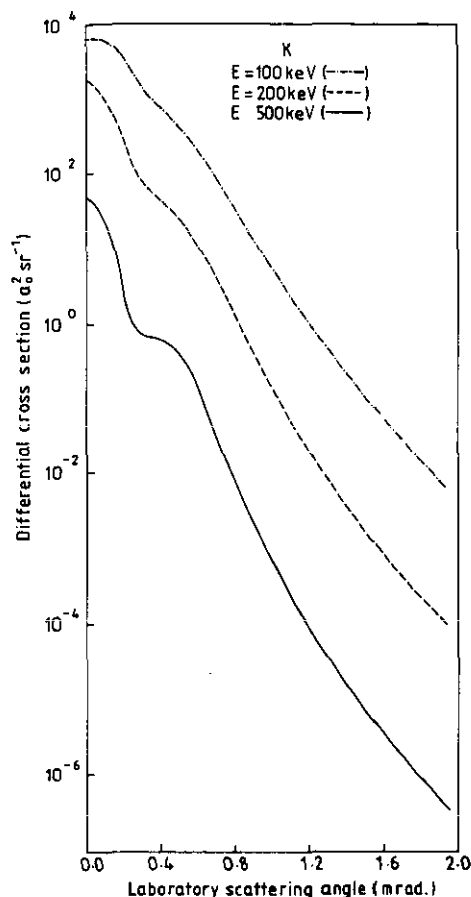
Figure 1. Differential cross sections for electron capture into the ground state of hydrogen in proton-potassium collisions at incident energies of 100, 200 and 500 keV.
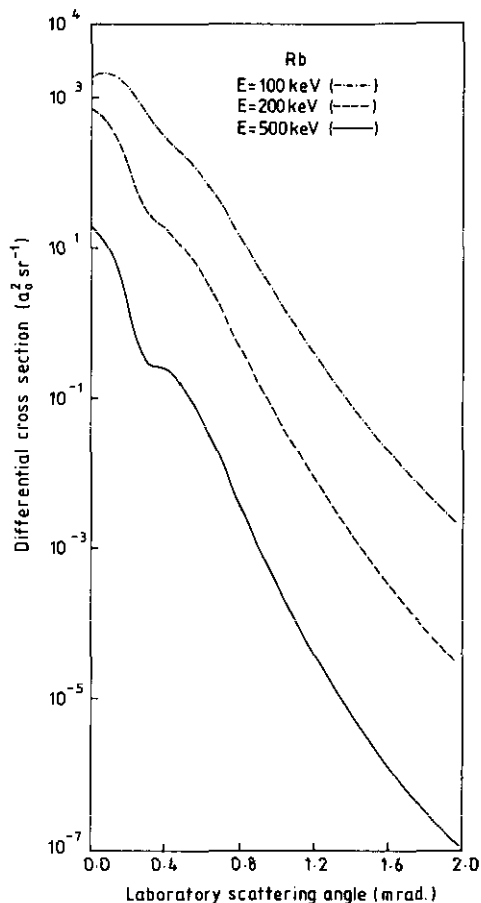
Figure 2. Differential cross sections for electron capture into the ground state of hydrogen in proton-rubidium collisions at incident energies of 100, 200 and 500 keV.

experimental measurement of these cross sections will provide helpful criteria in finding physically effective potentials and wavefunctions.

Figure 4 demonstrates the plots of differential cross sections against laboratory scattering angles for 2s and 2p state capture at an incident proton energy of 100 keV in the case of the proton–sodium and proton–potassium collisions. Figures 5 and 6 depict the corresponding results at incident proton energies of 200 and 500 keV, respectively. Figure 7 shows the results at incident proton energy of 100 keV for proton–rubidium and proton–caesium charge transfer reactions. Figures 8 and 9 depict the corresponding values at incident energies of 200 and 500 keV, respectively. The shapes of these curves and also the nature of the variation of the cross sections with energy and scattering angle show the same trend in the case of all the alkali-metal atoms. In general, the 2s capture cross sections are higher than the 2p state capture cross sections even though for a few small scattering angles the converse is the case. Hence it may be concluded that at a particular incident energy the general nature of the variation of the differential cross sections with scattering angle is independent of
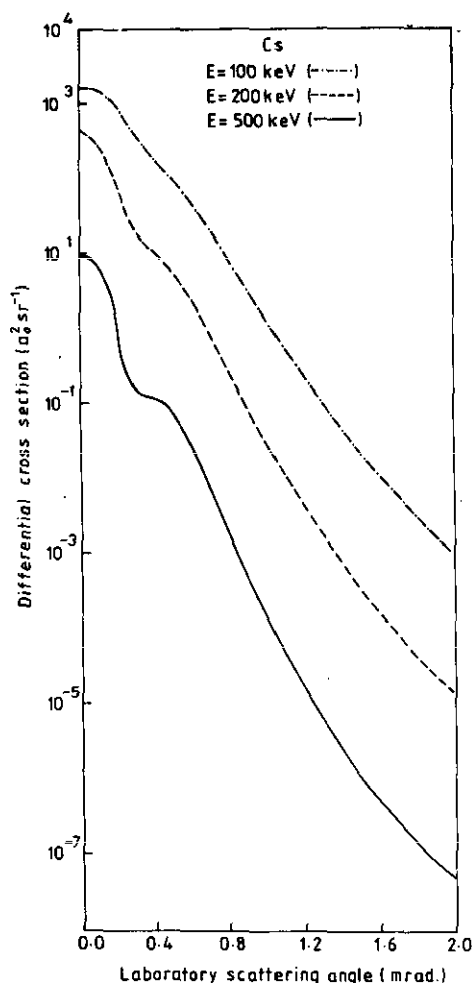
Figure 3. Differential cross sections for electron capture into the ground state of hydrogen in proton-caesium collisions at incident energies of 100, 200 and 500 keV.

the atomic mass number of the alkali-metal atom. It is interesting to note the existence of points of inflection or local extremum in the differential cross sections at a laboratory scattering angle of about 0.5 mrad. During the last few years there has been a considerable growth of interest in the possibility of the occurrence of a peak in the differential cross section for an electron capture process, a possibility which was suggested by the classical double-scattering mechanism proposed many years back by Thomas (1927). Thomas peaks have been observed for charge transfer in p–He and p–H collisions by Horsdal-Pedersen *et al* (1983) and Vogt *et al* (1986), respectively. While the angles at which these experimentally observed peaks occur are close to the angles at which we find the extrema in our proton–alkali-metal-atom charge transfer calculations, the Thomas peaks usually appear at considerably higher incident energies. We are inclined to attribute the occurrence at the local extrema in the calculated differential cross sections for electron capture from alkali-metal atoms mainly to the nature of the model potential used in (8*b*) and hope that future experiments will throw more light on the applicability of such potentials.

    The impulse approximation method is thus seen to turn out to be a convenient second-order method for studying valence electron capture from alkali-metal atoms.
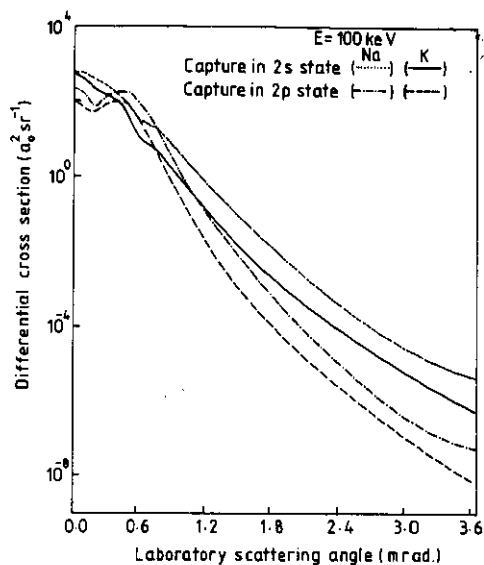
Figure 4. Differential cross sections for electron capture into the 2s and 2p states of hydrogen at an incident energy of 100 keV in proton–sodium and proton–potassium collisions.
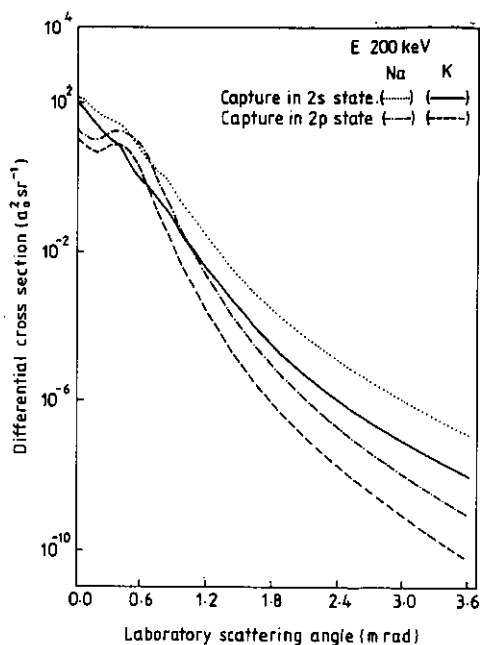

Figure 5. Differential cross sections for electron capture into the 2s and 2p states of hydrogen at an incident energy of 200 keV in proton–sodium and proton–potassium collisions.
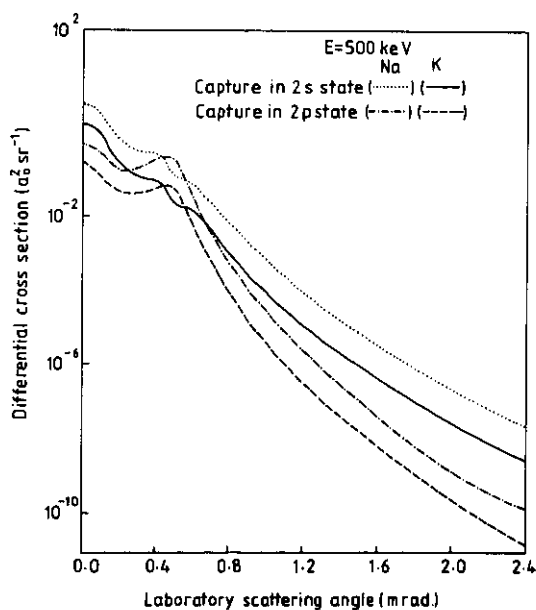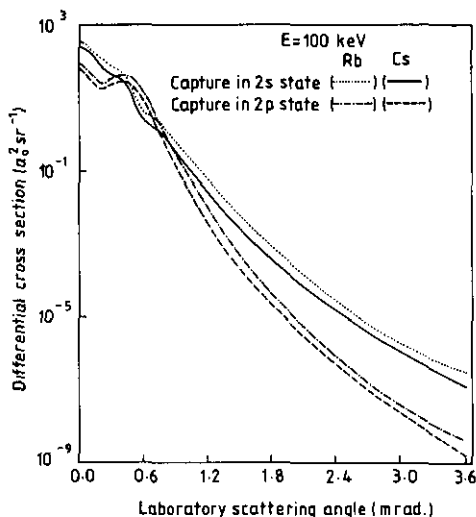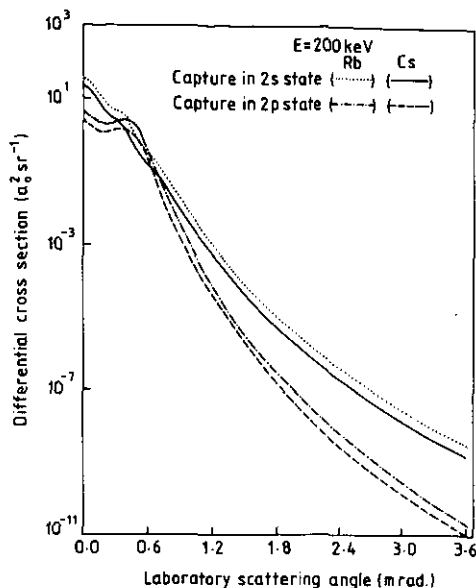

Figure 6. Differential cross sections for electron capture into the 2s and 2p states of hydrogen at an incident energy of 500 keV in proton–sodium and proton–potassium collisions.
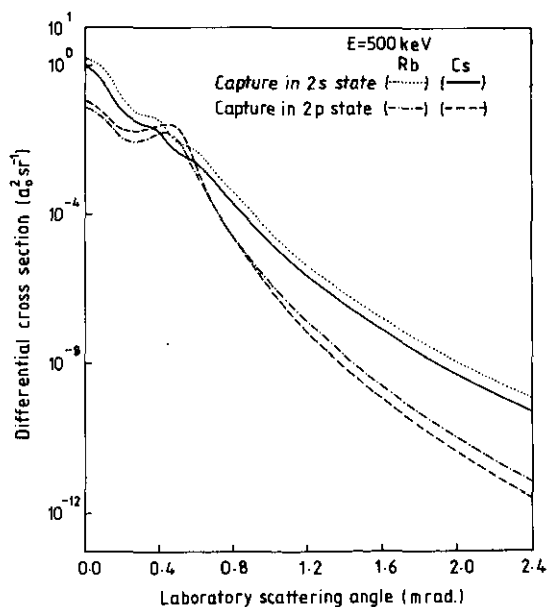
Figure 7. Differential cross sections for electron capture into the 2s and 2p states of hydrogen at an incident energy of 100 keV in proton–rubidium and proton–caesium collisions.

Figure 8. Differential cross sections for electron capture into the 2s and 2p states of hydrogen at an incident energy of 200 keV in proton–rubidium and proton–caesium collisions.

Figure 9. Differential cross sections for electron capture into the 2s and 2p states of hydrogen at an incident energy of 500 keV in proton–rubidium and proton–caesium atom collisions.

It may be used with advantage for determining the differential and integral cross sections for electron transfer to ground and excited states, although for excited state capture the analytical work is laborious and needs to be carefully planned.

Appendix

A.1. Evaluation of the integrals for ground state and 2s state capture

For the ground (1s) state of hydrogen

$$\varphi_{Af}(r_{1A}) = \varphi_{1s}(r_{1A}) = \frac{(aZ_A)^{3/2}}{\pi^{1/2}} \exp(-aZ_A r_{1A}) \tag{A1}$$

where $Z_A = 1$.

Substituting this $\varphi_{Af}(r_{1A})$ on the right-hand side of (13) of the text, and using Nordsieck's method (Nordsieck 1954) of working out integrals involving confluent hypergeometric functions (see also McDowell and Coleman 1970), we obtain

$$F_{1s}(q, t) = \int \varphi_{1s}^*(r_{1A}) \exp(it \cdot r_{1A})\,_1F_1(-i\nu_q; 1; (qr_{1A} - q \cdot r_{1A}))\, dr_{1A}$$

$$= -4\pi \frac{(aZ_A)^{3/2}}{\pi^{1/2}} \left(\frac{\partial}{\partial I} \frac{(I^2 + t^2)^{-i\nu_q - 1}}{[I^2 + t^2 - 2(iIq + t \cdot q)]^{-i\nu_q}} \right)_{I = aZ_A}. \tag{A2}$$

Using (A2) in (12b) of section 2, we obtain finally, after some simplification equation (15) of the text.

For the 2s excited state of hydrogen

$$\varphi_{Af}(r_{1A}) = \varphi_{2s}(r_{1A}) = \frac{(aZ_A)^{3/2}}{2\sqrt{2}\,\pi^{1/2}} (1 - \gamma r_{1A}) \exp(-\gamma r_{1A}) \tag{A3}$$

where

$$\gamma = \tfrac{1}{2}aZ_A.$$

After parametric differentiation and further simplification and also writing $T_G = \gamma^2 + t^2 = (\tfrac{1}{2}aZ_A)^2 + t^2$,

$$F_{2s}(q, t) = 8\pi^{1/2}\gamma^{3/2} \left(\frac{2\gamma(1 + i\nu_q)}{T_G^2} - \frac{2\gamma^3(1 + i\nu_q)(2 + i\nu_q)}{T_G^3} + \frac{(-i\nu_q)(2\gamma - iq)}{T_G[T_G - 2(i\gamma q + t \cdot q)]} \right.$$

$$\left. + \frac{4\gamma^2(1 + i\nu_q)(i\nu_q)(\gamma - iq)}{T_G^2[T_G - 2(i\gamma q + t \cdot q)]} + \frac{2\gamma(-i\nu_q)(\gamma - iq)^2(i\nu_q - 1)}{T_G[T_G - 2(i\gamma q + t \cdot q)]^2} \right)$$

$$\times \left(\frac{T_G}{T_G - 2(i\gamma q + t \cdot q)} \right)^{-i\nu_q}. \tag{A4}$$

Therefore the transition matrix element for the 2s state capture process is

$$T_{i2s} = -\frac{32 D\lambda_i a^3 \gamma^{3/2}}{\pi^{1/2}} \int \left(\frac{2\gamma(1 + i\nu_q)}{T_G^2} - \frac{2\gamma^3(1 + i\nu_q)(2 + i\nu_q)}{T_G^3} + \frac{(-i\nu_q)(2\gamma - iq)}{T_G[T_G - 2(i\gamma q + t \cdot q)]} \right.$$

$$\left. + \frac{4\gamma^2(1 + i\nu_q)(\gamma - iq)(i\nu_q)}{T_G^2[T_G - 2(i\gamma q + t \cdot q)]} + \frac{2\gamma(-i\nu_q)(\gamma - iq)^2(i\nu_q - 1)}{T_G[T_G - 2(i\nu q + t \cdot q)]^2} \right)$$

$$\times \left(\frac{T_G}{T_G - 2(i\gamma q + t \cdot q)} \right)^{-i\nu_q} N(\nu_q)$$

$$\times \left(\frac{1}{(t - q)^2} - \frac{A}{(t - q)^2 + \lambda^2 a^2} \right) P_1(q)\, dq. \tag{A5}$$

A.2. Evaluation of the integrals for 2p state capture

The integrals $F_{2p}(q, t)$ for the three final 2p states are first worked out by taking the 2p wavefunctions to be quantized with the direction of $\eta = t - q$ as the direction of the polar axis and the plane of η and t as the azimuthal reference plane. These are then transformed with the help of rotation matrices (Coleman and McDowell 1965, Coleman and Trelease 1968) to yield integrals corresponding to hydrogen 2p states quantized with the direction of t as the polar axis and the plane of t and k_i as the azimuthal reference plane. The 2p state wavefunctions of the hydrogen atom which refer to the rectangular coordinate reference frame are represented as

$$\varphi_{2p_z}(r_{1A}) = \frac{\gamma^{5/2}}{\pi^{1/2}} r_{1A} \exp(-\gamma r_{1A}) \cos \theta' \tag{A6a}$$

$$\varphi_{2p_x}(r_{1A}) = \frac{\gamma^{5/2}}{\pi^{1/2}} r_{1A} \exp(-\gamma r_{1A}) \sin \theta' \cos \Phi' \tag{A6b}$$

$$\varphi_{2p_y}(r_{1A}) = \frac{\gamma^{5/2}}{\pi^{1/2}} r_{1A} \exp(-\gamma r_{1A}) \sin \theta' \sin \Phi'. \tag{A6c}$$

Correspondingly, we write

$$F_{2p_{z(x,y)}}^{t}(q, t) = \int \varphi_{2p_{z(x,y)}}^{*}(r_{1A}) \exp(it \cdot r_{1A})$$

$$\times {}_1F_1(-i\nu_q; 1; i(qr_{1A} - q \cdot r_{1A})) \, dr_{1A} \tag{A7}$$

where the superscript t refers to the fact that the final 2p wavefunctions are quantized with the direction of t as the polar axis and the plane of t and k_i as the azimuthal reference plane. We shall denote by ν and ϕ the polar and azimuthal angle of q in this axis system. After carrying out a procedure similar to that described by Coleman and McDowell (1965) and further simplifying,

$$F_{2p_z}^{t}(q, t) = \left(\frac{\gamma^5}{\pi}\right)^{1/2} (16\pi i)\left(\frac{(1+i\nu_q)(2+i\nu_q)\gamma t}{T_G^3}\right.$$

$$+ \frac{(-i\nu_q)(1+i\nu_q)(2\gamma t - \gamma q \cos \nu - iqt)}{T_G^2[T_G - 2(i\gamma q + t \cdot q)]}$$

$$\left. + \frac{(-i\nu_q)(1-i\nu_q)(t - q \cos \nu)(\gamma - iq)}{T_G[T_G - 2(i\gamma q + t \cdot q)]^2}\right)$$

$$\times \left(\frac{T_G}{T_G - 2(i\gamma q + t \cdot q)}\right)^{-i\nu_q} \tag{A8a}$$

$$F_{2p_x}^{t}(q, t) = -\cos \varphi \left(\frac{\gamma^5}{\pi}\right)^{1/2} (16\pi i)(-i\nu_q)q \sin \nu \left(\frac{(1+i\nu_q)\gamma}{T_G^2[T_G - 2(i\gamma q + t \cdot q)]}\right.$$

$$\left. + \frac{(1-i\nu_q)(\gamma - iq)}{T_G[T_G - 2(i\gamma q + t \cdot q)]^2}\right)\left(\frac{T_G}{T_G - 2(i\gamma q + t \cdot q)}\right)^{-i\nu_q} \tag{A8b}$$

$$F_{2p_y}^{t}(q, t) = F_{2p_x}^{t}(q, t) \tan \varphi. \tag{A8c}$$

The transition matrix elements for the $2p_z$, $2p_x$ and $2p_y$ state capture processes are to

be determined by substituting the above expressions in the following integrals

$$T_{i2p_{z(x,y)}} = -\frac{4D\lambda_1 a^3}{\pi} \int F'_{2p_{z(x,y)}}(q, t) N(\nu_q) \left(\frac{1}{(t-q)^2} - \frac{A}{(t-q)^2 + \lambda^2 a^2}\right)$$

$$\times \left(\frac{1}{[(av+q)^2 + a^2\lambda_1^2]^2}\right) dq. \tag{A9}$$

The ϕ integration can be done analytically and it is found that the contribution from the $F'_{2p_y}(q, t)$ term is zero. The transition matrix elements T_{i2p_z} and T_{i2p_x} are then computed numerically by integrating over ν and q as described in section 2.1 of the text.

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