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The use of second order potentials in the theory of the scattering of charged particle by atoms
III. A four-channel approximation for electron and proton scattering by hydrogen atoms

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Abstract. The method of Bransden and Coleman (1972) is applied to scattering by hydrogen atoms in a four-channel approximation in which the 1s, 2s and 2p states are explicitly included. Results are given for 1s–2s and 1s–2p excitation by electrons and protons.

1. Introduction

The eigenfunction expansion method introduced by Bransden and Coleman (1972, to be referred to as Paper I) was applied to collisions of electrons and protons with hydrogen atoms in Paper II (Bransden *et al* 1972). The calculations were limited to the one- and two-channel versions of the theory, in the impact parameter formalism. In the present paper we again use the impact parameter formalism but now the 1s, 2s and 2p states are explicitly included in the expansion; this may be described as a four-channel approximation because, with a suitable choice of axes, the $2p_y$ state does not arise. The kernels of the resulting four coupled integrodifferential equations (see equation (5) of Paper II) contain matrix elements of the form

$$\int \frac{\phi^*_{nlm}(\boldsymbol{r})\phi_{n'l'm'}(\boldsymbol{r})}{|\boldsymbol{r}-\boldsymbol{x}|\,|\boldsymbol{r}-\boldsymbol{x}'|}\,\mathrm{d}\boldsymbol{r}$$

where $\phi^*_{nlm}(\boldsymbol{r})$ is a hydrogen wavefunction. These integrals, in which l and l' can be 0 or 1, were evaluated by the method described by Coleman (1972). As in our previous work, the effective energy parameter $\bar{\epsilon}$ was chosen so as to ensure that the leading term in the asymptotic expansion of the effective potential has the correct coefficient.

Cross sections were evaluated by using the equation

$$Q(1\mathrm{s}, n) = 2\frac{k_\mathrm{f}}{k_\mathrm{i}}\int_0^\infty |a_n(\infty)|^2 b\,\mathrm{d}b(\pi a_0^2) \tag{1}$$

a modified version of equation (2) of Paper II which takes account of the energy loss by the projectile. The factor $k_\mathrm{f}/k_\mathrm{i}$ arises in a natural way when equation (1) is derived from the wave treatment as in Paper I, rather than from the simple impact parameter approach involving the assumption of constant projectile velocity.

2. Electron impact

Cross sections calculated in the four-channel approximation are listed in table 1 and are compared with other results in figures 1, 2 and 3. The one- and two-channel results shown in the figures are the results of Paper II modified by the inclusion of the kinematic factor k_f/k_i.

Table 1. Cross sections (in units of πa_0^2) for electron impact. E is the electron energy in eV.

E	1s–2s	1s–2p
25	$2{\cdot}67^{-2}$	$9{\cdot}70^{-1}$
35	$3{\cdot}58^{-2}$	$1{\cdot}04$
54	$4{\cdot}40^{-2}$	$9{\cdot}55^{-1}$
70	$4{\cdot}43^{-2}$	$8{\cdot}81^{-1}$
100	$4{\cdot}00^{-2}$	$7{\cdot}36^{-1}$
200	$2{\cdot}60^{-2}$	$4{\cdot}75^{-1}$

The superscript indicates the power of 10 by which the number is to be multiplied.

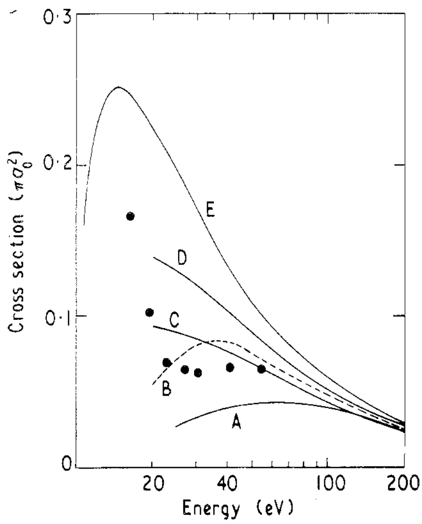

Figure 1. 1s–2s excitation by electrons. Curve A four-channel approximation (present work); curve B Glauber approximation (Tai *et al* 1970); curve C two-channel approximation (Paper II); curve D one-channel approximation (Paper II); curve E Born approximation. ● pseudo-state method (Burke and Webb 1970)

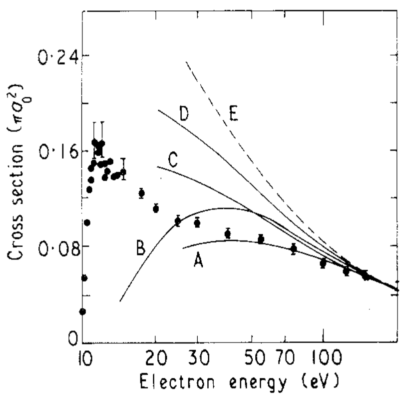

Figure 2. Q(1s–2s)$+0{\cdot}23Q$(1s–3p) for electron impact. Q(1s–3p) is evaluated in the one-channel approximation (Paper II). Curves A–E as in figure 1. ⧫ experimental results of Kauppila *et al* (1970)

The approximations of Paper II make no allowance for the coupling between the degenerate 2s and 2p states. The effect of this coupling on the 1s–2s cross section is evident from figure 1 and its inclusion brings our results for Q(1s–2s)$+0{\cdot}23\ Q$(1s–3p) into very close agreement with the measurements of Kauppila *et al* (1970) as shown in figure 2.

For the 1s–2p transition there is little difference between the one- and four-channel approximations and the calculations are still at variance with the experiments of Long *et al* (1968). In figure 4 the polarization fractions deduced from our four-channel calculations are compared with the measurements of Ott *et al* (1970). The two sets of results have the same shape but differ in magnitude, whereas both the Born approximation and the Glauber approximation (Gerjuoy *et al* 1972) agree quite closely with the measurements. If we had chosen the axis of quantization perpendicular to the momentum transfer, as suggested by Gerjuoy *et al* (1972), and then transformed the calculated differential cross sections to refer them to an axis of quantization in the direction of $\boldsymbol{k}_i$, it is to be expected that our results would be increased and brought into closer agreement with the polarization measurements. This transformation would not affect the total cross section for excitation of the 2p state.

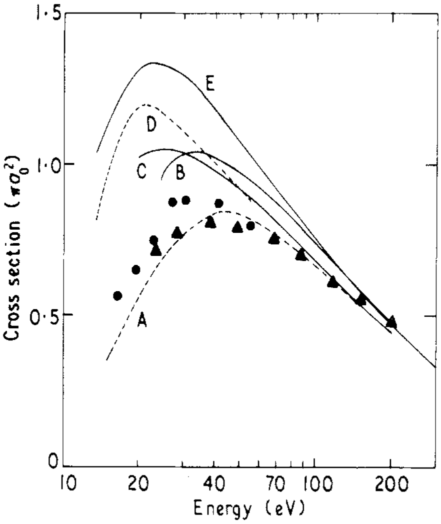

Figure 3. 1s–2p excitation by electrons. Curve A Glauber approximation (Tai *et al* 1970): curve B four-channel approximation (present work): curve C one-channel approximation (Paper II): curve D 1s–2s–2p close coupling approximation (Burke *et al* 1963): curve E Born approximation. ● pseudo-state method (Burke and Webb 1970); ▲ experimental results of Long *et al* (1968)

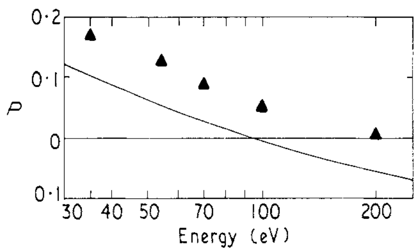

Figure 4. Polarization fraction P for 1s–2p excitation by electrons. Solid curve: four-channel approximation (present work). ▲ experimental results of Ott *et al* (1970).

The differential cross sections for elastic scattering in the one- and four-channel approximations differ by no more than a few per cent, but the differential cross sections for excitation to the $n = 2$ level obtained in the four-channel approximation are somewhat smaller than the one-channel results of Paper II. Detailed results are given elsewhere (Sullivan 1972).

3. Proton impact

Table 2 shows the four-channel results for excitation by protons. The influence of the 2s–2p coupling on the 1s–2s cross section is again evident from figure 5 where the difference between curves B and C is very much greater than that between curves A and B. The former difference is a consequence of explicit inclusion of the 2p state whereas the latter difference represents the effect of the allowance which our method makes for those states not explicitly included in the expansion.

In comparing figure 6, which shows the 1s–2p results, with figure 7 of Paper II it should be noted that in that figure the origin was inadvertently displaced on the vertical axis.

Table 2. Cross sections (in units of πa_0^2) for proton impact. E is the proton energy in keV

E	1s–2s	1s–2p
25	$4{\cdot}25^{-1}$	$8{\cdot}93^{-1}$
35	$4{\cdot}11^{-1}$	$8{\cdot}13^{-1}$
50	$3{\cdot}40^{-1}$	$8{\cdot}53^{-1}$
70	$2{\cdot}50^{-1}$	$8{\cdot}81^{-1}$
100	$1{\cdot}67^{-1}$	$8{\cdot}71^{-1}$
200	$7{\cdot}49^{-2}$	$6{\cdot}73^{-1}$

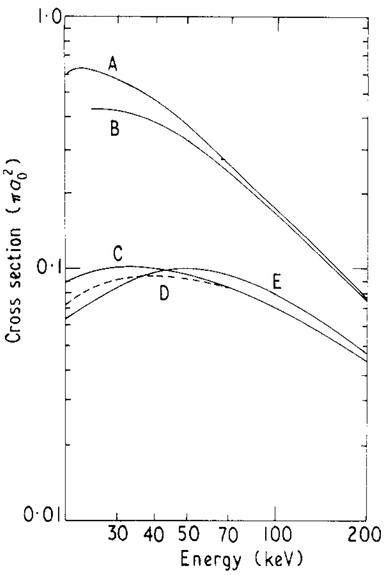

Figure 5. 1s–2s excitation by protons. Curve A four-state approximation (Flannery 1969); curve B four-channel approximation (present work); curve C two-channel approximation (Paper II); curve D one-channel approximation (Paper II); curve E Glauber approximation (Franco and Thomas 1971).

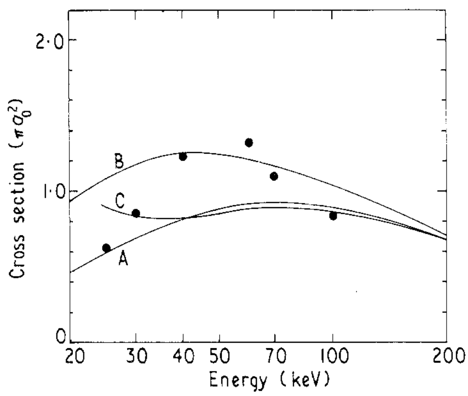

Figure 6. 1s–2p excitation by protons. Curve A Glauber approximation (Franco and Thomas 1971); curve B one-channel approximation (Paper II); curve C four-channel approximation (present work). ● pseudo-state approximation (Cheshire *et al* 1970).

4. Conclusion

The work described here removes an unsatisfactory feature of our earlier work, as the 2s and 2p states are now treated in the same way. Comparison with the results of Paper

II reveals the substantial influence of the coupling between the 2s and 2p states (see also Damburg and Propin 1972). Our four-channel results for 1s–2s excitation by electrons are in very close agreement with the measurements of Kauppila *et al* (1970) except at the lower end of our energy range where the effect of electron exchange is no longer negligible.

The significance of the rearrangement channels in the case of proton impact was mentioned in § 8 of Paper II. An indication of their effect is obtained by comparing the results obtained by Flannery (1969) with those of Cheshire *et al* (1970), as the former took account of the 1s, 2s and 2p states of the target whereas the latter included the same states of both target and projectile. The closeness of our results to those of Flannery (1969) serves to emphasize the desirability of including some of the rearrangement channels explicitly in our model.

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