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LETTER TO THE EDITOR

A pseudostate multichannel eikonal study of e–H(1s) inelastic collisions

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Abstract. The effect of including the $3\bar{s}$ and $3\bar{p}$ pseudostates is examined for the 2s and 2p excitation of atomic hydrogen by incident electrons with energy E (eV) in the range $16{\cdot}5 \leqslant E \leqslant 200$. The 2s excitation is most strongly affected and displays a behaviour consistent with measurement and refined theories which include polarization. The 2p excitation agrees particularly well with the full quantal pseudostate treatment and with experiment. A seven-channel (1s, 2s, 2p, 3s, 3p) treatment is also performed, and the resulting 2s and 2p cross sections lie closer to those of the pseudostate description than to the four-channel (1s, 2s, 2p) results, as expected.

In this letter, the multichannel eikonal approach (Flannery and McCann 1975) is examined for the excitations,

$$e+H(1s) \rightarrow e+H(2s, 2p, 3s, 3p) \tag{1}$$

in which the $3\bar{s}$ and $3\bar{p}$ pseudostates of Burke and Webb (1970) are explicitly acknowledged. In this treatment, the amplitude for scattering with final relative momentum $\boldsymbol{k}_f$ in direction (θ, ϕ) with respect to polar axis along the direction of incident relative momentum $\boldsymbol{k}_i$ is, in the CM frame,

$$f_{if}(\theta, \phi) = -i^{\Delta+1}\int_0^\infty J_\Delta(K'\rho)[I_1(\rho,\theta)-iI_2(\rho,\theta)]\rho\, d\rho \tag{2}$$

where J_Δ are Bessel functions of integral order, and where K' is the XY component $k_f \sin\theta$ of the momentum change $\boldsymbol{K} = \boldsymbol{k}_i - \boldsymbol{k}_f$. The collision functions

$$I_1(\rho,\theta;\alpha) = \int_{-\infty}^{\infty} \kappa_f(\rho, Z)\left(\frac{\partial C_f(\rho, Z)}{\partial Z}\right) \exp(i\alpha Z)\, dZ \tag{3}$$

and

$$I_2(\rho,\theta;\alpha) = \int_{-\infty}^{\infty}\left(\kappa_f(\kappa_f-k_f)+\frac{\mu}{\hbar^2}V_{ff}\right)C_f(\rho, Z)\exp(i\alpha Z)\, dZ \tag{4}$$

contain a dependence on the scattering angle θ via

$$\alpha = k_f(1-\cos\theta) = 2k_f\sin^2(\tfrac{1}{2}\theta) \tag{5}$$

the difference between the Z component of the momentum change $\boldsymbol{K}$ and the minimum change $k_i - k_f$ in the collision. The coupling amplitudes C_f are solutions of the following set of N coupled differential equations

$$\frac{\mathrm{i}\hbar^2}{\mu}\kappa_f(\rho, Z)\frac{\partial C_f(\rho, Z)}{\partial Z}+\left(\frac{\hbar^2}{\mu}\kappa_f(\kappa_f-k_f)+V_{ff}(\rho, Z)\right)C_f(\rho, Z)$$
$$=\sum_{n=1}^{N} C_n(\rho, Z)V_{fn}(\rho, Z)\exp \mathrm{i}(k_n-k_f)Z, \qquad f=1,2,\ldots,N \tag{6}$$

solved subject to the boundary condition $C_f(\rho, -\infty)=\delta_{if}$. The local wavenumber of relative motion at separation $\boldsymbol{R}\equiv(R,\Theta,\Phi)\equiv(\rho,\Phi,Z)$ is

$$\kappa_n(\boldsymbol{R})=\left(k_n^2-\frac{2\mu}{\hbar^2}V_{nn}(\boldsymbol{R})\right)^{1/2}$$

where the interaction matrix elements

$$V_{nm}(\boldsymbol{R})=\langle\phi_n(\boldsymbol{r})|V(\boldsymbol{r},\boldsymbol{R})|\phi_m(\boldsymbol{r})\rangle$$

connect the various electronic states $\phi_n(\boldsymbol{r})$ describing the isolated systems and where $V(\boldsymbol{r},\boldsymbol{R})$ is the instantaneous electrostatic interaction.

The present description has automatically included an infinite number of partial waves of relative motion which are distorted by the static interactions associated with the various channels included in the basis set expansion and which in turn are coupled to the internal electronic motions via the amplitudes C_f in (6). Moreover in contrast to previous semiclassical descriptions† explicit account is taken of the variation during the collision of the different local momenta of relative motion in each channel.

Close-coupling calculations have been performed by using (2)–(6) in which the 1s, 2s, $2\mathrm{p}_{0,\pm1}$ states of atomic hydrogen are included together (*a*) with the $3\bar{\mathrm{s}}$ and $3\bar{\mathrm{p}}$ pseudostates of Burke and Webb (1970) introduced to acknowledge couplings to all higher open channels and (*b*) with the actual 3s and 3p atomic states. In tables 1 and 2 are displayed total excitation cross sections

$$\sigma_f(E)=2\pi\frac{k_f}{k_i}\int|f_{if}(\theta,\phi)|^2\,\mathrm{d}(\cos\theta) \tag{7}$$

for processes (1) at incident electron energy E (eV). Previous four-channel results F for the 2s and 2p excitations (Flannery and McCann 1975) converge from above and below

Table 1. Total cross sections (πa_0^2) given by a four-channel treatment F, and two seven-channel treatments (P and R, with and without pseudostates, respectively) of $\mathrm{e}+\mathrm{H(1s)}\rightarrow\mathrm{e}+\mathrm{H(2s\ or\ 2p)}$ at electron energy E (eV).

nl	2s			$2\mathrm{p}_0$	$2\mathrm{p}_{\pm1}$	2p		
E	F	P	R	P	P	F	P	R
16·5	—	0·151	0·112	0·405	0·125	—	0·530	0·600
20	0·145	0·127	0·124	0·481	0·224	0·720	0·705	0·730
30	0·124	0·095	0·115	0·485	0·379	0·836	0·864	0·863
50	0·090	0·074	0·088	0·421	0·466	0·865	0·887	0·881
100	0·052	0·048	0·052	0·227	0·421	0·629	0·648	0·645
200	0·028	0·027	0·028	0·120	0·338	0·453	0·458	0·454

† Compare Flannery and McCann (1974) when $I_2=0$, $\kappa_f=k_f$ in (3) and (6) and the coefficient of C_f in the left-hand side of (6) is neglected, and also Bransden (1970).

Table 2. Total cross sections (0·01 πa_0^2) given by seven-channel treatment of $e+H(1s) \rightarrow e+H(nl)$; nl = 3s, $3p_0$, $3p_{\pm 1}$, at electron energy E (eV).

E \ nl	3s	$3p_0$	$3p_{\pm 1}$	3p
16·5	1·41	5·04	2·19	7·23
20	1·78	6·67	4·23	10·9
30	1·87	7·25	7·52	14·8
50	1·46	5·65	8·96	14·6
100	0·90	3·13	8·00	11·1
200	0·50	1·61	5·81	7·42

respectively onto the pure seven-channel treatment R. Addition of the pseudostates in P considerably distorts the shape and changes the magnitude of the 2s excitation while σ_{2p} remains relatively unaffected. Replacing the pseudostates by the real 3s and 3p states in general yields cross sections which lie between F and P although closer to P, as expected.

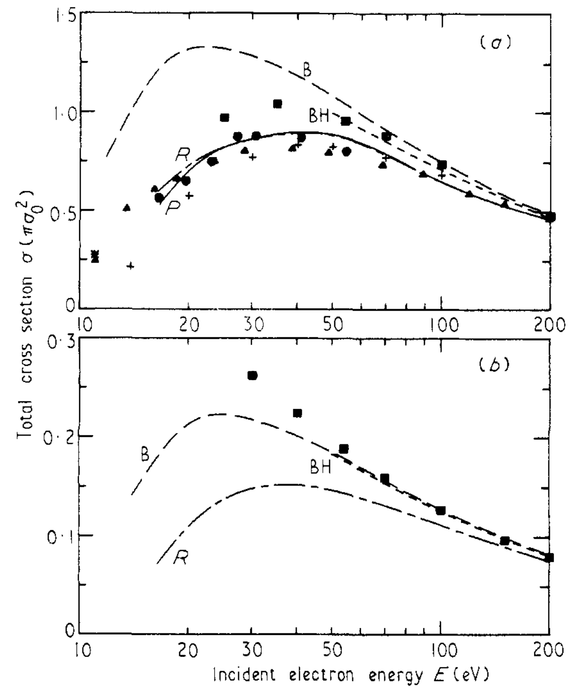

Figure 1. Cross sections (πa_0^2) for (*a*) the 2p and (*b*) the 3p excitations from H(1s) by electrons with energy E (eV). P and R are the present seven-channel results with pseudo and real 3s and 3p states respectively. Experiment: ▲ (Long *et al* 1968), * (Williams and Willis 1974); theory: ● pseudostate (Burke and Webb 1970), second-order potential method: ■ (*a*) four-channel approximation (Sullivan *et al* 1972), (*b*) one-channel approximation (Bransden *et al* 1972), + Glauber approximation (Tai *et al* 1970), BH Baye and Heenen (1974), B Born approximation.

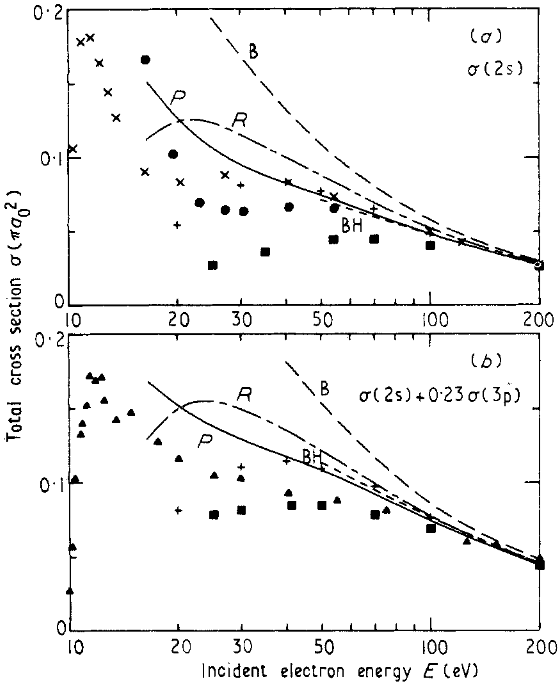

Figure 2. Cross sections for the 2s excitation from H(1s) by electrons with energy E (eV). Notations as in figure 1, except experiment: ▲ Kauppila *et al* (1970), theory: × McDowell *et al* (1974).

These effects are further illustrated in figures 1 and 2 where comparison theoretical and experimental data are provided. In figure 1(*a*), the 2p measurements of Long *et al* (1968) are normalized to the present F value at 200 eV (rather than to the Born section which is 7% higher). The recent absolute measurement of Williams and Willis (1974) at 11 eV is 13% higher than the corresponding 2p cross section of Long *et al.* The present σ_{2p} are in very good agreement with the experiment and with the fully quantal pseudostate treatment of Burke and Webb. The recent twenty-state second-order diagonalization impact-parameter description of Baye and Heenen (1974) for the 2p and 3p excitations, in figure 1, is in close accord with the second-order potential treatment of Bransden *et al* (1972) and Sullivan *et al* (1972), an approach based on the impact-parameter method, and designed to acknowledge couplings with all excited states. Born and Glauber (cf Tai *et al* 1970) cross sections are also included in the figures.

In figure 2, the main effect of pseudostate addition causes the 2s cross section to continue its increase as the impact energy E is reduced to 16·5 eV, reflecting a behaviour also exhibited by the treatments of Burke and Webb, and of McDowell *et al* (1973). This behaviour is real and is consistent with the measurements shown in figure 2(*b*) of Kauppila *et al* (1970) who estimate a cascade contribution of 0·23 σ_{3p} to the observed 2s excitation. The present 3s cross sections are shown in figure 3 together with other theoretical values, for comparison.

Rather than presenting all the differential cross sections, from which σ_f in (7) were obtained, it suffices to report that the 2p scattering did not depart appreciably from the earlier study (Flannery and McCann 1975). In figure 4, the pseudostates reduce the

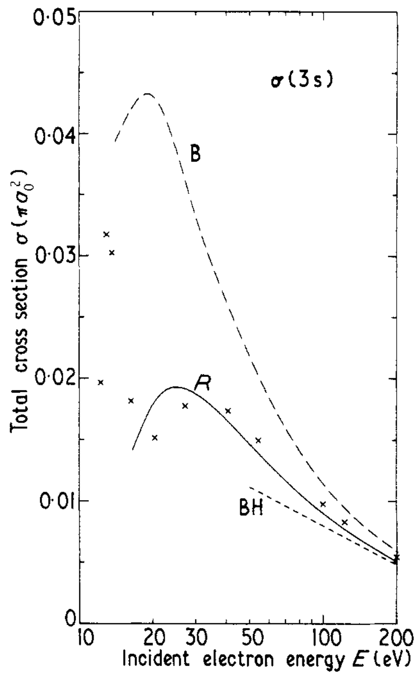

Figure 3. Cross sections (πa_0^2) for the 3s excitation from H(1s) by electrons with energy E (eV). Notation as in figure 2 with ×, McDowell *et al* (1973).

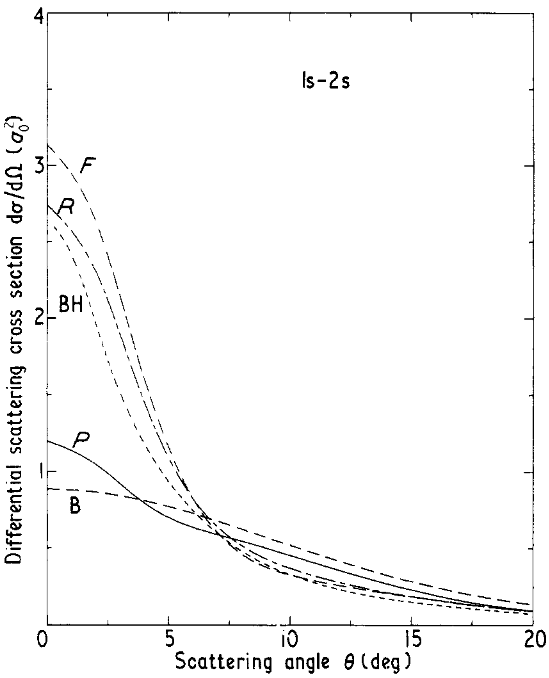

Figure 4. Differential cross sections for 2s excitation from H(1s) at 100 eV impact energy. Notation as in figure 1 with F: four-channel treatment (Flannery and McCann 1975).

2s scattering at 100 eV in the forward direction and enhance the scattering through larger angles, the net result being a slight increase in the total cross section at 100 eV. This behaviour becomes increasingly amplified as the impact energy E is reduced and figures similar to 4 are available upon request.

In contrast, pseudostates increase the four-channel elastic scattering in the forward direction as expected since the potential appropriate to the distant elastic encounters becomes more long range. Hence, agreement with the experiment of Teubner *et al* (1973) became somewhat improved for small-angle scattering. However, because of the neglect of electron exchange needed for a proper description of closer encounters, the present treatment still failed (Flannery and McCann 1975) to provide a good description (cf Winters *et al* 1974) of elastic scattering through the larger scattering angles.

In conclusion, addition of pseudostates does improve the agreement for inelastic collisions of the present multichannel eikonal approach with experiment and with other refined theories which include polarization effects. In particular, the continuing rise of σ_{2s} as E is reduced to below about 20 eV is consistent with experiment (cf figure 2*b*), although, at these low energies, electron exchange is important and could cause the required reduction needed to improve accord between the present approach and experiment (cf figure 2*b*).

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