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2S-excitation of atomic hydrogen by electrons at intermediate energies

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Abstract. The method of Das developed recently to analyse elastic scattering of electrons by atoms has been extended in the present paper to inelastic scatterings. The method has been applied for the computation of 2S-excitation, cross-sections at two typical intermediate energies *viz.* 54.4 eV and 100 eV energies. Some of the results are compared with available experimental results and are found to be in satisfactory agreement with these.

Keywords. Elastic scattering; inelastic scattering; 2S-excitation; electron; positron; hydrogen; Born-amplitude; differential cross-section.

1. Introduction

Recently a simple computational procedure has been suggested by Das (Das 1979; Das *et al* 1981; Das and Biswas 1981) for the calculation of scattering cross-sections of electrons by atoms. The method has already been used for electron-hydrogen (Das and Biswas 1980) and electron-helium (Das 1979; Das *et al* 1981) elastic scattering for intermediate energies. The overall results are observed to be very good except for one or two points. Naturally it will be interesting to extend the method for inelastic scatterings and observe the accuracy of the results. In this context it may be recalled that the well-known calculational methods like the DWSBA method (Kingston and Walters 1980) and the EBS method (Byron and Latour 1976) do not give very accurate results for the excitational calculation of hydrogen atoms by electrons for intermediate energies. Here we consider the 2S-excitation of atomic hydrogen by electron impact. The calculational method we follow needs the second order Born amplitudes. Byron and Latour presented an approximate set of results for the second Born amplitude for 100 eV energy. Recently Ermolaev and Walters (1980) also presented an exact set of results for the second Born amplitude at 54·4 eV energy. In our present calculation we make use of the above two sets of results to obtain the 2S-excitation cross-section results.

2. Computational method

In electron atom scatterings the direct amplitudes are the on-shell values of the

T-matrix element which satisfy an infinite set of coupled integral equations (Das *et al* 1981; Das and Biswas 1981).

$$T_{ni} = T^B_{ni} + \sum_I \int d^3 p_I \, T^B_{nI} \frac{1}{E - E_I + i\epsilon} T_{Ii}. \tag{1}$$

Similar set of equations may be written in connection with the exchange amplitudes. Now the essence of the computational method of Das is to solve the set of equations (1) approximately by the least squares method (Delves and Walsh 1974). In choosing the trial set one may again use (1) and pick up important contributions in its right side. For elastic scattering it turns out that a simple choice of the trial input T-matrix elements is

$$T^{(\mathrm{in})}_{ni} = [a(E) + i\, b(E)]\, T_{ni}, \tag{2}$$

where $(a + ib)$ is a certain energy dependent complex variational parameter to be determined so as to make the sum of the squares of the residuals a minimum. For the optimal values of the parameter so determined the output values of T_{fi} on the energy shell give the direct amplitude. For inelastic scattering, such as in the $2S$-excitation of atomic hydrogen, it will be interesting to see how the results behave when a similar choice is made for the set of input T-matrix element. Once such a choice is made the bulk of the computation rests in computing the second Born amplitude. Recently, Ermolaev and Walters (1980) published exact second Born amplitudes for $2S$-excitation at 54·4 eV energy. Byron and Latour (1976) also presented a set of approximate second Born amplitudes for 100 eV energy. We use these two sets of results and compute the scattering cross-sections for the $2S$-excitation for the above two energies which are two typical energies in the intermediate range. The exchange amplitude has been calculated in two different ways. One is the usual Ochkur (1963) approximation and the other is the Ochkur-Das approximation (Das and Biswas 1980). Results of our computation are presented in § 3 and are compared with some other theoretical results and with some experimental results.

3. Results

The differential cross-sections at the energies 54·4 and 100 eV, with the exchange amplitudes calculated in the Ochkur and Ochkur-Das approximation are approximately the same. For the elastic scattering this is not the case, however. See in this connection table 2 where we present results of a computation following Das which use the exact second Born amplitudes of Ermolaev and Walters (1979) and use the exchange amplitude of the above two approximations (Das and Biswas 1980) for 30 eV energy. For the elastic scattering the Ochkur-Das approximation gives, in general, better results particularly at smaller angles where the cross-sections are considerably large and dominate the total cross-section results. It may be remarked that the computational method of Das gives fairly good results for the elastic scattering case specially with the exact second Born amplitudes.

In figures 1 and 2 and table 1, we compare our results for the differential cross-sections for the $2S$-excitation of atomic hydrogen with the results of some other theories for 54·4 and 100 eV energies and with the only available experimental results of Williams (1981) for 54·4 eV. In these figures we also present the results of the first and second Born approximation. For small angles, say for less than 20°, there exist considerable differences among the various calculated results, particularly for 54·4 eV. For 54·4 eV our results show a deep within 10° scattering angle. This is absent in the results of other calculations. The measured values of Williams are available from 10° onwards. Moreover, their results are marked by large uncertainties and even more serious is the fact that their measured values (labelled (i) and (ii) in table 1) following two different procedures gives significantly different results in this small angle region. One of these measured values for 10° compare favourably with the close coupling calculations of Kingston *et al* (1976) while the other one favours the DWSBA results of Kingston and Walters (1980) and the latter result is about 3/2 times the results of the present calculation. The same is nearly true for 20°. The first and second Born results are considerably large in this small angle region. For 100 eV energy results of all these calculations come closer beyond 10°. But within 10° our results show a depression, not shown in other results. For this energy EBS results of Byron and Latour (1976) are also available (figure 2). These agree with those of other calculations.

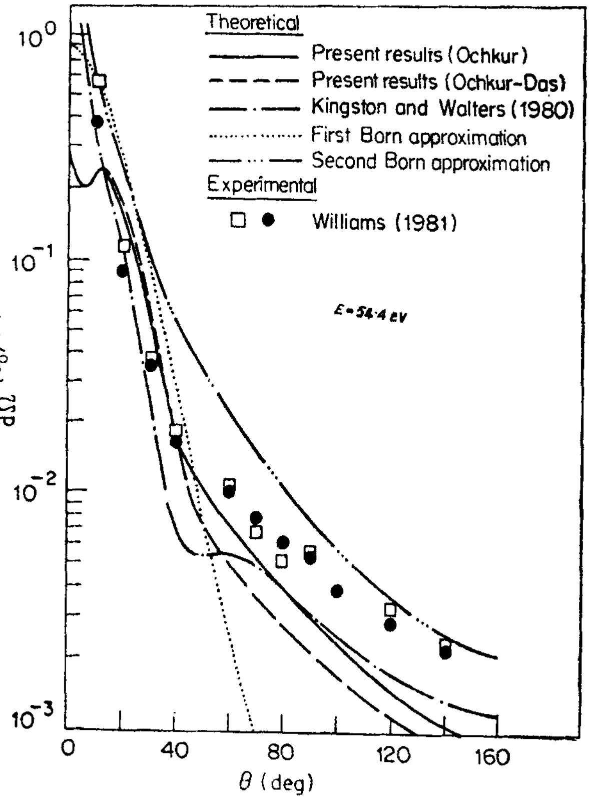

Figure 1. Differential cross-sections for $1S$–$2S$ excitation of atomic hydrogen by electron impact at 54.4 eV energy.

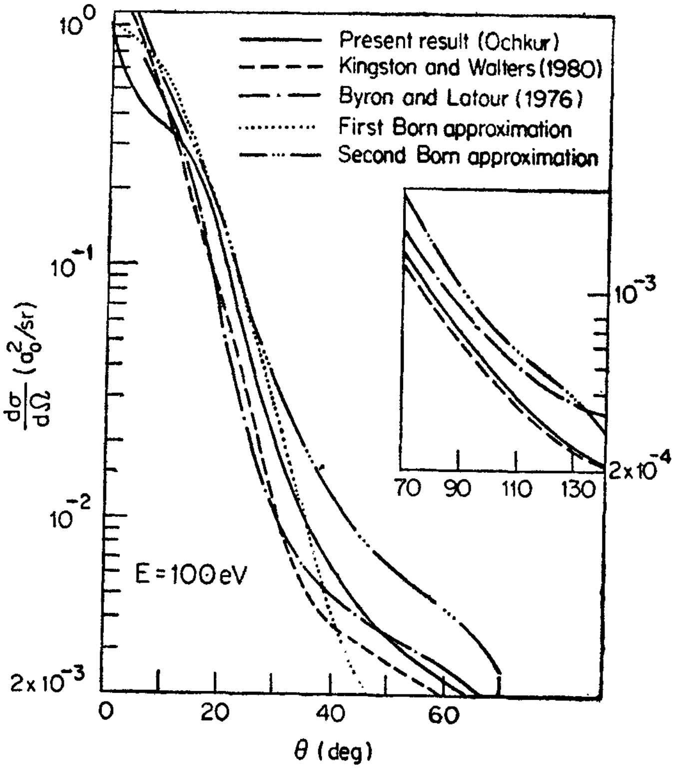

Figure 2. Differential cross-sections for 1*S*–2*S* excitation of atomic hydrogen by electron impact at 100 eV energy.

For intermediate angles, say extending from 20° to 90°, except the first and second Born results, the other available results are close to each other, with the exception that around 40°, the DWSBA results show prominent depression, particularly for 54·4 eV. The present results for 54·4 eV energy agree fairly with the measurements of Williams. If we look to table 1 and see results from small to large angles it will appear that the close coupling calculation of Kingston *et al* (1976) is in best agreement with the experimental results of Williams (1981). But this raises some controversy since it is already known (Kingston and Walters 1980, table 7) that the total 2*S*-excitation cross-section results of Kingston and Walters are roughly twice the previous experimental results (Kauppila *et al* 1970). So more experimental results, both differential and total, are needed to clarify the situation. For intermediate angles we expect our results to be fairly good. This is partly supported by the experimental result at 54·4 eV and partly from the results for the $(2s+2p)$ excitation. This support comes from the fact that the results for $(2s+2p)$ excitation of Kingston and Walters underestimate the experimental values by nearly the same percentage by which their 2*S*-excitation results fall short of the present result, except around 40°. Here one may expect that the results for $2p$ excitation following the present method will be of similar accuracy as those for 2*S*-excitation. In any case the present results for intermediate angles may be considered fairly good.

Finally we consider the large angle result, say for angle greater than 90°. Here our results best agree with the DWSBA results of Kingston and Walters. Both the results

Table 1. Differential cross-sections ($a_0^2\,\mathrm{sr}^{-1}$) for $1S$–$2S$ excitation of the atomic hydrogen by electron impact for 54·4 and 100 eV energies.

Angle (deg)	54·4 eV						100 eV		
	Kingston *et al* (1976)	Kingston and Walters (1980)	Present calculation (Ochkur exchange	Present calculation (Ochkur Das exchange)	Experimental results of Williams (1981)		Kingston *et al* (1976)	Kingston and Walters (1980)	Present calculation (Ochkur exchange)
					(i)	(ii)			
10	0·575	0·333	0·224	0·233	0·380 (128)†	0·594 (94)	0·365	0·368	0·359
20	0·123	0·110	0·170	0·178	0·090 (18)	0·116 (17)	0·0881	0·0746	0·104
30	0·0443	0·0270	0·0580	0·0612	0·035 (39)	0·0375 (40)	0·0200	0·0103	0·0186
40	0·0190	0·0069	0·0190	0·0174	0·0165 (128)	0·0184 (47)	0·00759	0·00376	0·0062
50	0·0124	0·0055	0·0103	0·0074	—	—	0·00433	0·00275	0·0033
60	0·0099	0·0056	0·0075	0·0050	0·0101 (48)	0·0106 (31)	0·00274	0·00195	0·0023
70	0·0082	—	0·0054*	0·0037*	0·0079 (34)	0·00704 (218)	0·00184	—	0·0015
75	—	0·0045	0·0048	0·0033	—	—	—	0·00109	—
80	0·0066	—	0·0041*	0·0028*	0·00615 (247)	0·00527 (163)	0·00128	—	0·00097
90	0·0054	0·0032	0·0031	0·0022	0·00543 (117)	0·00570 (128)	0·00093	0·00064	0·00067
120	0·0033	0·0017	0·0015	0·0012	0·00282 (98)	0·00321 (114)	0·00047	0·00029	0·00030
140	0·0028	0·00135	0·0011	0·0009	0·00218 (87)	0·00224 (87)	0·00036	0·000215	0·00022

*Interpolated from computed values at other points

†the numbers in the brackets are two standard deviation errors in the last digits (we apprehend a few printing errors in the numbers within the brackets which are corrected here)

Table 2. Differential cross-sections (a_0^2 sr^{-1}) for elastic scattering of electrons by hydrogen atom for 30 eV energy. Present calculation uses the exact second Born amplitude of Ermolaev and Walters (1979).

Angle (deg)	Fon *et al* (1978)	Kingston and Walters (1980)	Fon *et al* (1981)	Das and Biswas (1980)	Present (Ochkur exchange)	Present (Ochkur-Das exchange)	Williams (1975) (Expt.)
5	—	—	7·59	5·98	6·65	7·80	—
10	4·74	8·58	5·63	4·46	4·82	5·70	5·32
20	2·44	5·30	2·95	2·25	2·58	3·00	2·74
30	1·36	3·44	1·63	1·29	1·56	1·70	1·60
60	0·437	0·495	0·437	0·369	0·473	0·460	0·461
90	0·213	0·160	0·189	0·146	0·162	0·167	0·162
120	—	0·088	0·108	0·073	—	—	0·105
140	0·111	0·071	0·090	0·053	0·054	0·061	0·091

of close coupling calculations and the EBS calculations are pretty large in this angular range. Here again the close coupling calculation favours the experimental results of Williams. The first Born results are too small while the second Born results appear to be better.

Next we consider the results for total cross-sections for the 2*S*-excitation at these two energies. We find that our computed values 0·0618 πa_0^2 at 54·4 eV and 0·045 πa_0^2 at 100 eV energies compare favourably with the experimental results of Kauppila *et al* (1970) (0·056 ± 0·004) πa_0^2 and (0·039 ± 0·004) πa_0^2 at 54·4 and 100 eV energies respectively. The corresponding DWSBA results of Kingston and Walters are 0·0537 πa_0^2 and 0·0404 πa_0^2. The first Born results at these energies are 0·102 πa_0^2 and 0·057 πa_0^2 respectively and the close coupling calculation of Kingston *et al* are 0·101 πa_0^2 and 0·0582 πa_0^2 respectively. The above comparisons give enough evidence that the computational method of Das works nicely for inelastic scatterings as well.

4. Conclusions

The present study clearly indicates that the computational method suggested by Das is not only successful in describing elastic scatterings, it is also successful in describing inelastic scatterings. More experimental results, particularly for differential cross-sections, are warranted for a more clear understanding of the mechanism of inelastic scatterings and also about the usefulness of various calculational schemes.

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