Electron-Hydrogen Elastic Scattering at Intermediate and High Energies

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Abstract

Electron-hydrogen elastic scattering at intermediate and high energies (in the range 30-400 eV) is considered. The calculational method of Das is applied with improved input functions. Improvement is noticed in the results and, except around an energy of 100 eV, reasonable agreement is obtained with experiment.

1. Introduction

In a series of works Das and his associates reported a method of dealing with problems of elastic scattering of electrons by atoms at intermediate and high energies (see e.g. Das 1979; Das and Biswas 1980, 1981; Das *et al.* 1981). Previously, a set of results on electron-hydrogen scattering, calculated following the method of Das, was published (Das and Biswas 1980) for lower energies only, namely for 20, 30 and 50 eV, and the results were found to be very good. For very high energies the results are also very good. However, in the intermediate energy range, particularly at small angles, the results are not as good and are very similar in accuracy to the pseudo-state calculation of Fon *et al.* (1978). Now, with a view to improve upon the earlier calculation of Das and Biswas (1980), we undertake in the present work to take recourse in more flexible trial input functions containing more variational parameters. As we will see, this throws light also on some aspects of the calculational method of Das and suggests ways of further improving the results.

We may recall in this context that all other well known calculational methods have limited applicability. Thus the EBS calculation of Byron and Joachain (1977) is valid only for higher energies, say above 50 eV. In this region also the agreement with experiment is not uniformly good at all scattering angles. The same is also true for the DWSBA calculation of Kingston and Walters (1980). The most recent *R*-matrix calculation of Fon *et al.* (1981) appears to be more successful for lower energies, although it seems to have only a limited validity as well.

2. Theory

The direct scattering amplitude in electron-atom elastic collisions may be obtained from the on-shell values of the *T*-matrix element $T_{1s,1s}$, the off-shell values of which are related to other off-shell *T*-matrix elements by the set of integral equations (see Das *et al.* 1981)

$$T_{ni} = T_{nI}^{B} + \sum_{I} \int d^{3}p_{I} T_{ni}^{B} \frac{1}{E - E_{I} + i\eta} T_{Ii}.$$
 (1)

$$\sum_{n} \int |T_{ni}^{(\text{out})} - T_{ni}^{(\text{in})}|^2 \,\mathrm{d}\Omega \,. \tag{2a}$$

In this integral the on-shell values appear and a considerable simplification results if only one term in (2a) is retained (see Das and Biswas 1981):

$$\int |T_{1s,1s}^{(\text{out})} - T_{1s,1s}^{(\text{in})}|^2 \,\mathrm{d}\Omega.$$
(2b)

The outputs with the estimated parameters give the desired results.

It was observed in the work of Das and Biswas (1980) that a good choice for the T-matrix elements is

$$T_{ni}^{(in)} = \{a(E) + ib(E)\}T_{ni}^{B} \quad (\text{for all } n),$$
(3)

where a(E) and b(E) are two variational parameters. This calculation in which two variational parameters enter is termed a two-parameter calculation.

Now we turn to the exchange amplitude, which is exactly given by (see Das and Biswas 1980 for notation)

$$f_{\rm ex} = -4\pi^2 \langle \Phi_{\rm ex} | V_{\rm ex} | \psi_i^+ \rangle. \tag{4}$$

We note that the corresponding direct amplitude is given by

$$f_{\rm d} = -4\pi^2 \langle \Phi_{\rm f} | V | \psi_i^+ \rangle. \tag{5}$$

In equations (4) and (5) the same scattering state $|\psi_i^+\rangle$ appears. We seek an approximation to this state to use in computing both the direct and exchange amplitudes. In the two-parameter calculation we employ the approximation

$$f_{\rm d} \approx -4\pi^2 \langle \Phi_{\rm f} | V | (a_{\rm min} + {\rm i} \, b_{\rm min}) \Phi_i \rangle, \qquad (6)$$

where $(a_{\min} + i b_{\min}) \Phi_i$ gives a good representation of ψ_i^+ , except at large distances where, of course, both V and V_{ex} are very small. So in an approximate calculation of f_{ex} one may replace ψ_i^+ in (4) by the above expression to obtain

$$f_{\rm ex} \approx f_{\rm ex}^{\rm MBO} = (a_{\rm min} + i b_{\rm min}) f_{\rm ex}^{\rm BO}, \qquad (7)$$

where f_{ex}^{BO} is the Born-Oppenheimer (BO) approximation. The result (7) is termed the modified Born-Oppenheimer (MBO) exchange. Further, on replacing f_{ex}^{BO} by the usual high energy Ochkur (1964) approximation, one gets the Ochkur-Das (OD) approximation

$$f_{\rm ex}^{\rm OD} = (a_{\rm min} + i b_{\rm min}) f_{\rm ex}^{\rm Och} \,. \tag{8}$$

In previous calculations Ochkur and OD exchange have been used and, in the present paper, in addition to these we have also used MBO exchange.

The results obtained with the two-parameter calculation of the direct amplitude and with the Ochkur or improved OD approximation for the exchange are found to be good. Obviously with such a simple choice for the trial input set one cannot Electron-Hydrogen Elastic Scattering

expect the results to agree with experiment at all energies and all angles. Earlier calculations showed that the two-parameter results are good at both the lower and upper ends of the intermediate energy range, say for 20 or 30 eV and for 200 eV and above. Between 30 and 200 eV, however, considerable discrepancies remain.

In the present calculation the second Born term needed is evaluated approximately following the procedure of Byron and Joachain (1973), with a mean excitation energy $\Delta = 0.5$ a.u. This approximation, no doubt, produces some errors which are not insignificant at lower energies. This is evident from the comparison made in Table 1 (see Section 3) of the results of Das and Biswas (1980) with those obtained using the exact second Born amplitude of Ermolaev and Walters (1979) and with the experimental work of Williams (1975). However, one is unlikely to get a significant improvement by merely using an improved or even an exact second Born amplitude for energies such as 50 or 100 eV. At these energies the calculation itself needs improvement. One way of doing this is to use a more flexible trial input set, and this is the motivation of the present work.

An obvious choice for a more flexible trial input set is

$$T_{1s,1s}^{(in)} = \{a_1(E) + ib_1(E)\}T_{1s,1s}^{B},$$
(9a)

$$T_{n,1s}^{(in)} = \{a_2(E) + ib_2(E)\}T_{n,1s}^{B} \quad (n \neq 1s).$$
(9b)

The corresponding calculation we refer to as the four-parameter calculation. This calculation improves the results only marginally. There is a significant improvement only at higher energies and at large angles, but for intermediate energies such as 50 or 100 eV the small angle results and even more seriously the imaginary parts of the amplitudes significantly deteriorate. Now, it is not difficult to find reasons for such a deterioration (see Section 3). Thus, with a view to improving the results at 50 or 100 eV, we undertake a six-parameter calculation, choosing an input set as follows:

$$T_{1s,1s}^{(in)}(\boldsymbol{p}-\boldsymbol{k}_{i};\varepsilon_{0},\varepsilon_{0}) = (a_{1}+ib_{1})T_{1s,1s}^{B}(\boldsymbol{p}-\boldsymbol{k}_{i};\varepsilon_{0},\varepsilon_{0}) +a_{3}\frac{\mu^{4}}{\{(\boldsymbol{p}-\boldsymbol{k}_{i})^{2}+\mu^{2}\}^{2}} + ia_{4}\frac{\nu^{4}}{\{(\boldsymbol{p}-\boldsymbol{k}_{i})^{2}+\nu^{2}\}^{2}}, \quad (10a)$$

$$T_{n,1s}^{(in)}(\boldsymbol{p}-\boldsymbol{k}_{i};\varepsilon_{n},\varepsilon_{0}) = (a_{2}+ib_{2})T_{n,1s}^{B}(\boldsymbol{p}-\boldsymbol{k}_{i};\varepsilon_{n},\varepsilon_{0}) \quad (n \neq 1s).$$
(10b)

The reasons for such a choice will be discussed in the following section.

3. Results and Discussion

In a calculation with two parameters the output amplitude may be considered to have two parts, i.e. the first Born amplitude and the second Born amplitude multiplied by a complex variational parameter. For lower energies, say 30 eV, these two parts are equally important and have more or less a similar dependence on the scattering angle, and so the least squares method works nicely and yields good results for the scattering cross sections. As soon as an additional set of parameters is introduced in the four-parameter calculation to make the trial set more flexible the output breaks into three parts, i.e. the first Born amplitude, the second Born amplitude with a contribution from the intermediate ground state multiplied by the complex variational parameter $a_1 + i b_1$, and the second Born amplitude with contributions from the remaining intermediate states multiplied by the other complex variational parameter $a_2 + i b_2$. These last two parts have a drastically different analytical behaviour at intermediate energies. In fact the third part is highly peaked towards the forward direction, dominating at small angles and falling off rapidly at large angles. In the four-parameter calculation there is no term in the input $T_{1s,1s}^{(in)}$ with analytic behaviour comparable with this part of the output. Consequently, the least squares calculation cannot in this case produce the correct behaviour at small angles. The lack of stability of the least squares method is probably the reason for this incorrect behaviour. The situation is reminiscent of one in which use of orthogonal polynomials gives better results than a combination of simple powers in some simple variational calculations.



Fig. 1. Comparison of the second order Born contribution to the differential cross section (solid curve) from all intermediate states, other than the ground state, with the terms $\kappa^4/\{(k_t - k_i)^2 + \kappa^2\}^2$ for different values of $\kappa = \mu$, v at 100 eV: (a) the real part and (b) the imaginary part.

In a variational calculation for scattering problems the choice of a good trial function is a difficult problem. It is also the most crucial one. Even in a simple phase shift calculation for potential scattering by well known variational principles such as those of Kohn, a bad choice of the trial function may lead to absurd results (see e.g. Rudge 1973). Thus the lack of stability and the lack of precise guidelines are some of the serious problems of our calculational method, and these are shared by almost all other variational principles for scattering problems. Under these circumstances what can be done is to add some compensating terms to the ones already tried and see whether the input and output have similar analytical behaviour. In this way one may obtain better results.

We adopt this approach to improve the results at 50 and 100 eV, where the twoand four-parameter calculations are unsatisfactory. It should be noted here that both the real and imaginary parts of $T_{1s,1s}$, which are strongly varying with angle, can be represented by terms like $\kappa^4/\{(\mathbf{k}_f - \mathbf{k}_i)^2 + \kappa^2\}^2$ (see Fig. 1) for intermediate energies and for a suitable choice of the parameter κ . So for an improved calculation at 50 and 100 eV we make the choice given by equations (10). From the comparison made in Fig. 1 for the strongly varying terms in the output with the last two terms in (10a), it is reasonable to assume $\mu^2 = 4 \cdot 0$ and $v^2 = 0 \cdot 6$ at 100 eV. We have made the same choice for 50 eV, though for other energies other values will be appropriate. Even with this choice the real part is poorly represented at small angles and the imaginary part at large angles. The effects of this are reflected in the results.

Table 1.	Differential cross sections of four-parameter calculation compared with other results	for								
electron-hydrogen elastic scattering at low and high energies										

The	differential	cross	sections	are i	n units	s of	$a_0^2 {\rm sr}^2$	-1;	the	notation	a^n	represents	$a \times 10^{n}$	and	the
numbers in parentheses are uncertainties in the last digits															

Angle (deg.)	Kingston & Walters (1980)	Fon <i>et al.</i> (1981)	Ermo Walter Och. exch.	laev & s (1979) ^A OD exch.	Das & Biswas (1980) ^B	Present work (Och. exch.)	Williams (1975) (exp.)
				30 eV			<u></u>
10	8.58	5.63	4.82	5.70	4 46	2.49	5.32 (57)
20	5.30	2.95	2.58	3.00	2.25	2.06	2.74 (28)
30	3.44	1.63	1.56	1.70	1.29	1.59	1.60 (18)
60	4.95^{-1}	$4 \cdot 37^{-1}$	4.73-1	$4 \cdot 60^{-1}$	$3 \cdot 69^{-1}$	5.73-1	$4 \cdot 61^{-1}(52)$
90	1.60^{-1}	1.89-1	$1 \cdot 62^{-1}$	1.67^{-1}	$1 \cdot 46^{-1}$	$2 \cdot 25^{-1}$	$1 \cdot 62^{-1}(17)$
120	8.79-2	1.08^{-1}			$7 \cdot 25^{-2}$	$1 \cdot 20^{-1}$	$1 \cdot 28^{-1}(10)$
140	$7 \cdot 13^{-2}$	8.95-2	$5 \cdot 40^{-2}$	6·10 ⁻²	$5 \cdot 33^{-2}$	$9 \cdot 26^{-2}$	$9 \cdot 10^{-2}(9)$
				200 eV			
10	1.05			200 07	7·79 ⁻¹	$8 \cdot 61^{-1}$	
20	3.86^{-1}				$3 \cdot 53^{-1}$	$3 \cdot 79^{-1}$	$4 \cdot 19^{-1}(40)$
30	$1 \cdot 50^{-1}$				$1 \cdot 46^{-1}$	$1 \cdot 53^{-1}$	$1.72^{-1}(17)$
60	1.65^{-2}				$1 \cdot 63^{-2}$	$1 \cdot 80^{-2}$	$1.87^{-2}(19)$
90	$4 \cdot 35^{-3}$				$4 \cdot 50^{-3}$	$5 \cdot 14^{-3}$	$5 \cdot 84^{-3}(61)$
120	1.97^{-3}				$2 \cdot 20^{-3}$	$2 \cdot 47^{-3}$	$2 \cdot 72^{-3}(35)$
140	$1 \cdot 40^{-3}$				$1 \cdot 60^{-3}$	$1 \cdot 85^{-3}$	$1.78^{-3}(26)$
				400 eV			
10	$6 \cdot 13^{-1}$				$5 \cdot 66^{-1}$	5.93-1	
20	1.69^{-1}				1.70-1	1.70-1	$1.96^{-1}(21)$
30	$5 \cdot 10^{-2}$				$5 \cdot 17^{-2}$	$5 \cdot 14^{-2}$	$6 \cdot 17^{-2}(62)$
60	$4 \cdot 46^{-3}$				$4 \cdot 68^{-3}$	$4 \cdot 71^{-3}$	$4 \cdot 38^{-3}(62)$
90	$1 \cdot 13^{-3}$				$1 \cdot 26^{-3}$	$1 \cdot 28^{-3}$	$1 \cdot 04^{-3}(24)$
120	5.06-4				5.89-4	6.01-4	6.03-4(122)
140	3.66-4				4.34-4	4.44-4	5.06-4(115)

^A Two-parameter calculation with exact second Born amplitudes.

^B Two-parameter calculation with OD exchange.

The results of our four-parameter variational calculation are presented for lower (30 eV) and higher energies (200 and 400 eV) in the intermediate range in Table 1 and for some intermediate values (50 and 100 eV) in Table 2. We compare our results with the DWSBA results of Kingston and Walters (1980), the *R*-matrix results of Fon *et al.* (1981) and the experimental results of Williams (1975). The results are also compared in Table 1 with the two-parameter calculation of Das and Biswas (1980). (Here there was a minor programming error and so corrected results are used whenever reference to this calculation is made.) As already noted, we have tried in this calculation three different approximations for the exchange. For energies of

50 eV and above the Ochkur exchange and OD exchange give nearly identical results for the differential cross sections, although the two exchange terms differ considerably in phase. The MBO approximation gives significantly different cross sections at large angles (these last results are not shown in the tables). In fact for intermediate energies, say 50 or 100 eV, the Ochkur approximation (or the OD approximation) slightly overestimates the experimental results at large angles, while the MBO approximation slightly underestimates the results at these angles. With an increase of energy all these exchange amplitudes lead to nearly identical differential cross sections. From the results shown in Table 1, it is clear that for higher energies, say 200 or 400 eV, the agreement of our four-parameter results with experiment is good over the whole angular range, and better than the DWSBA results of Kingston and Walters (1980) or those of Byron and Joachain (1977) (not shown). Incidentally, it may be noted that our results agree quite closely with those of a pure static exchange. For energies of 50 or 100 eV, the present results are again better at large angles, but at small angles the agreement is not so good. Here the results are even inferior to the twoparameter calculation; the reasons for this have already been discussed.

 Table 2. Differential cross sections of two-, four- and six-parameter calculations compared with other results for electron-hydrogen elastic scattering at intermediate energies

The differential cross sections are in units of $a_0^2 \operatorname{sr}^{-1}$; the notation a^n represents $a \times 10^n$ and the numbers in parentheses are uncertainties in the last digits

Angle	Fon	Kingston	Fon		Williams			
(deg.)	<i>et al.</i> (1978)	& Walters (1980)	<i>et al.</i> (1981)	2P (Och. exch.)	4P (Och. exch.)	6P (Och. exch.)	6P (OD exch.)	(1975) (exp.)
			·	50 eV				
10	2.69	5.09	3.83	2.40	1.76	3.84	4·16	5.04 (51)
20	1 · 19	2.26	1.69	1.10	1 · 28	1.61	1.72	2.17 (23)
30	6.80-1	1.08	$8 \cdot 68^{-1}$	6.68-1	$8 \cdot 55^{-1}$	$8 \cdot 35^{-1}$	$8 \cdot 45^{-1}$	1.12 (12)
60	1.97-1	$1 \cdot 82^{-1}$	1.98^{-1}	$1 \cdot 83^{-1}$	$2 \cdot 21^{-1}$	1.97-1	$1 \cdot 92^{-1}$	$2 \cdot 05^{-1}(19)$
90	$7 \cdot 32^{-2}$	$5 \cdot 72^{-2}$	$7 \cdot 12^{-2}$	5.67-2	7.70-2	$6 \cdot 21^{-2}$	6.31-2	$7 \cdot 16^{-2}(82)$
120	$3 \cdot 57^{-2}$	$2 \cdot 92^{-2}$	$3 \cdot 69^{-2}$	$2 \cdot 59^{-2}$	3.99-2	$2 \cdot 88^{-2}$		$3 \cdot 49^{-2}(33)$
140	$2 \cdot 58^{-2}$	$2 \cdot 23^{-2}$	$2 \cdot 84^{-2}$	1.89-2	$3 \cdot 06^{-2}$	$2 \cdot 10^{-2}$	$2 \cdot 21^{-2}$	$2.73^{-2}(26)$
				100 eV				
10	1.41	2.22		1-21	1.22	1.87	1.94	
20	6·71 ⁻¹	8.46-1		$6 \cdot 05^{-1}$	$7 \cdot 15^{-1}$	7.36-1	$7 \cdot 42^{-1}$	1.10 (10)
30	$3 \cdot 71^{-1}$	3.83-1		3.39-1	$3 \cdot 82^{-1}$	3.66-1	$3 \cdot 62^{-1}$	$5 \cdot 09^{-1}(49)$
60	7.08^{-2}	$5 \cdot 62^{-2}$		$5 \cdot 58^{-2}$	6·40 ⁻²	$5 \cdot 61^{-2}$	$5 \cdot 63^{-2}$	$7 \cdot 22^{-2}(71)$
90	$2 \cdot 09^{-2}$	$1 \cdot 62^{-2}$		$1 \cdot 57^{-2}$	$1 \cdot 96^{-2}$	$1 \cdot 50^{-2}$	$1 \cdot 52^{-2}$	$2 \cdot 09^{-2}(20)$
120	$9 \cdot 5^{-3}$	7·6 ⁻³		7·4 ⁻³	9.8-3	6·7 ⁻³		$9 \cdot 2^{-3}$ (9)
140	6.8-3	$5 \cdot 6^{-3}$		$5 \cdot 5^{-3}$	7.4-3	$4 \cdot 8^{-3}$	4·9 ⁻³	$6 \cdot 5^{-3}$ (7)

^A Results for the present calculation with two, four or six parameters.

Next we consider the results of the six-parameter calculation. We have already seen that the two- and four-parameter calculations together describe satisfactorily the experimental results at lower and higher energies in the intermediate range. Our six-parameter calculation is designed to match the experimental results for several energies in the intermediate range, say 50 and 100 eV, where the two- and four-parameter results are not in conformity with experiment. The six-parameter results are displayed in Table 2, where for the exchange amplitude we use the Ochkur or

OD approximations. Comparison with experimental (Williams 1975) and other theoretical work shows that the overall trend of the present results is good, although these appear to fall rather rapidly at large angles. It is again observed that OD exchange (which is the same as MBO exchange at these angles) gives better results at small angles. The disagreement that still remains is partly due to the form of the compensating terms (we recall here that the imaginary part falls off rather too fast at large angles while the real part rises rather too slowly at small angles). In any case, the agreement for 50 eV may be considered satisfactory, while the results for 100 eV appear to be unsatisfactory. Part of this disagreement may be due to experimental errors for this energy, however, this needs further confirmation. It may be mentioned in this context, that the six-parameter calculation depends sensitively on the choice of the parameters μ^2 and ν^2 (see equation 10a). An incorrect choice of for example μ^2 too small or ν^2 too large may lead to very poor results, a consequence of the lack of stability of the calculational method already mentioned.

Perhaps for an accurate and stable calculation one may have to consider scattering in several channels jointly, analogous to a close-coupling calculation where some sort of feedback mechanism is adopted for continuous improvement of the results; for example, by the introduction of suitable compensating terms in the input, on the basis of observation of the outputs.

4. Conclusions

It is found that the two-parameter calculation gives results which are good at the lower and upper ends of the intermediate energy range and at higher energies for electron-hydrogen elastic scattering. The four-parameter calculation only marginally improves the results, except at higher energies where the improvement is significant. The inclusion of compensating terms then leads to satisfactory results from low to high energies. There remains some scope for improving the calculation still further.

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