J. Phys. B: At. Mol. Phys. **14** (1981) 2657–2665. Printed in Great Britain

Elastic scattering of electrons by hydrogen and helium atoms at intermediate and high energies

J N Das and N Saha

Department of Applied Mathematics, University College of Science, 92 Acharya Prafulla Chandra Road, Calcutta-700 009, India

Received 30 December 1980, in final form 20 March 1981

Abstract. Electron–hydrogen and electron–helium elastic scattering problems have been studied from an asymptotic analysis of the off-shell amplitudes. The resulting differential and total cross sections are observed to agree nicely with the experimental results and with the most elaborate theoretical calculations, such as the many-body theory employing the Hartree–Fock Green's function for electron–helium scattering and the pseudostate calculation of Fon, Burke and Kingston for electron–hydrogen scattering, over wide energy ranges.

1. Introduction

That the set of integral equations for the off-shell scattering amplitudes could be a starting point for a good theoretical calculation has been shown by Das and his associates in a series of works (see Das 1979, Das *et al* 1981, Das and Biswas 1980, 1981, Saha 1980). For elastic scattering an asymptotic analysis of the integral equations shows that the off-shell amplitudes have simple asymptotic forms. These asymptotic forms were used earlier to choose suitable trial input sets of amplitudes for solving the integral equations by the least-squares method. The results obtained are always found to be very good, agreeing well with the experimental results and the results of other very elaborate calculations, such as the many-body theory with Hartree–Fock Green's function calculation of Scott and Taylor (1979a, b), the eikonal Born series calculations of Byron and Joachain (1977), the second-order potential model calculation of Winters *et al* (1974), the distorted-wave second Born calculation of Buckley and Walters (1974) and Dewangan and Walters (1977) for elastic electron–helium scattering and the pseudostate calculation of Fon *et al* (1978) and the eikonal Born series calculation of Byron and Joachain (1977) for elastic electron–hydrogen scattering.

It was observed by Das (see Das *et al* 1981) that the off-shell amplitudes are approximately asymptotic to the corresponding Born elements multiplied by a complex, energy-dependent parameter. Furthermore this complex parameter has an integral representation in terms of the elastic scattering amplitude. It will naturally be interesting to evaluate approximately the corresponding integral and see how these values of the parameter agree with the optimal set of values obtained by the least-squares method. This is attempted in the present paper. With the parameters thus obtained the on-shell scattering amplitudes and the differential and total cross sections for elastic electron–hydrogen and electron–helium scattering have been computed.

0022-3700/81/152657+09$01.50 © 1981 The Institute of Physics

The exchange effects have been taken into account by the Ochkur approximation and the Ochkur–Das approximation (see Das and Biswas 1980). The results for differential cross sections are observed to be very good and, except at small angles, the results using the Ochkur–Das approximation are always better.

2. Theory

The off-shell T-matrix elements for the direct elastic electron–atom scattering satisfy the set of integral equations (see Das *et al* 1981)

$$T_{ni}(\boldsymbol{k}_n, \boldsymbol{k}_i; \varepsilon_n, \varepsilon_i) = T^{\mathrm{B}}_{ni}(\boldsymbol{k}_n, \boldsymbol{k}_i; \varepsilon_n, \varepsilon_i) + \sum_I \int \mathrm{d}^3 p_I T^{\mathrm{B}}_{nI}(\boldsymbol{k}_n, \boldsymbol{k}_I; \varepsilon_n, \varepsilon_I) \frac{1}{E - E_I + \mathrm{i}\eta} T_{Ii}(\boldsymbol{k}_I, \boldsymbol{k}_i; \varepsilon_I, \varepsilon_i) \tag{1}$$

where T_{nm} in these equations stands, in general, for the off-shell T-matrix element for the transition from the state 'm' to the state 'n' and the corresponding element with superscript 'B' stands for the first Born element. The arguments $(\boldsymbol{k}_n, \varepsilon_n)$ stand respectively for the momentum of the electron and the bound-state energy of the atom in the state 'n'. For scattering from the ground state, 'i' is to be replaced by '0'. Now let us investigate the asymptotic form of the T-matrix elements $T_{n0}(\boldsymbol{k}_n, \boldsymbol{k}_i; \varepsilon_n, \varepsilon_0)$ for $|\boldsymbol{k}_n| \to \infty$. Since, in general, $T^{\mathrm{B}}_{nI}(\boldsymbol{k}_n, \boldsymbol{k}_i; \varepsilon_n, \varepsilon_I)$ vanishes much faster than $T^{\mathrm{B}}_{n0}(\boldsymbol{k}_n, \boldsymbol{k}_i; \varepsilon_n, \varepsilon_0)$ for all $I \neq 0$, we obtain as a good approximation

$$T_{n0}(\boldsymbol{k}_n, \boldsymbol{k}_i; \varepsilon_n, \varepsilon_0) \sim (a(E) + \mathrm{i}b(E)) T^{\mathrm{B}}_{n0}(\boldsymbol{k}_n, \boldsymbol{k}_i; \varepsilon_n, \varepsilon_0) \tag{2}$$

where

$$a(E) + \mathrm{i}b(E) = 1 + \int \mathrm{d}^3 p_I \frac{T_{00}(\boldsymbol{k}_I, \boldsymbol{k}_i; \varepsilon_0, \varepsilon_0)}{E - \frac{1}{2}k_I^2 - \varepsilon_0 + \mathrm{i}\eta}. \tag{3}$$

A set of T-matrix elements which have the approximate asymptotic behaviour will be a good choice as the input set for the least-squares calculation, since the large k behaviour in the momentum space is linked with the small r behaviour in the coordinate space. One may therefore try to estimate the parameters a and b from equation (3) with a suitable approximation for T_{00} and use these in equation (2) to find an input set of T-matrix elements, ultimately substituting these in equation (1) in order ot obtain the output amplitudes. The on-shell values of these give the required scattering amplitudes. The main difficulty in using equation (3) for estimating the values of a and b lies in finding a suitable approximation for T_{00}. The first, simple, choice may be to replace T_{00} by the Born value T^{B}_{00} but this is expected to give results far from the actual values. Surprisingly, however, the values obtained for b agree nicely with the optimal values calculated by the least-squares principle. We give an explanation for the agreement in the following section. The next choice may be to replace T_{00} in equation (3) by the asymptotic value $(a(E) + \mathrm{i}b(E)) T^{\mathrm{B}}_{00}$. Then, identifying the two sides of equation (3), we obtain

$$a = \frac{(1 - t_{\mathrm{R}})}{(1 - t_{\mathrm{R}})^2 + t_{\mathrm{I}}^2} \tag{4}$$

$$b = \frac{t_I}{(1 - t_{\mathrm{R}})^2 + t_{\mathrm{I}}^2} \tag{5}$$

where

$$t_R + it_I = \int d^3p_I \frac{T_{00}^B(\boldsymbol{k}_I, \boldsymbol{k}_i; \varepsilon_0, \varepsilon_0)}{E - \frac{1}{2}k_I^2 - \varepsilon_0 + i\eta}. \tag{6}$$

We name the values of a and b thus obtained as the self-consistent values. The integration appearing in equation (6) may be analytically performed for the case of hydrogen. The results are given by

$$t_R = \frac{1}{k_i}(\tan^{-1} k_i - \pi) + \frac{1}{2(1+k_i^2)} \tag{7}$$

and

$$t_I = \frac{1}{2k_i}\left(1 + \log(1+k_i^2) - \frac{1}{1+k_i^2}\right). \tag{8}$$

Similar results may be obtained in the case of the helium atom when the helium wavefunction is chosen in simple form, for example those taken by Byron and Joachain (1973). Finally the direct part of the scattering amplitude will be given by

$$f_d = (f_{B_1} + af_{B_2R} - bf_{B_2I}) + i(af_{B_2I} + bf_{B_2R}). \tag{9}$$

For the exchange amplitude we take the Ochkur approximation result and also the Ochkur–Das (see Das and Biswas 1980) approximation, namely

$$f_{ex}^{OD} = (a + ib) f_{ex}^{Och}. \tag{10}$$

The differential cross sections and the total cross sections are then calculated and are presented and discussed in the following section.

3. Results

We have applied the analysis of the last section in computing the differential cross sections for the elastic scattering of electrons by hydrogen and helium atoms over wide energy ranges. In this computation the first and second Born direct amplitudes are needed. The second Born amplitudes have been evaluated in the usual way by taking the effect of the intermediate ground state exactly and the effect of the rest by a closure relation. For the mean excitation energy we choose $\Delta = 0.5$ au for the hydrogen atom and $\Delta = 1.3$ au for the helium atom (see in this context Byron and Joachain 1973, 1977). The values of a and b are obtained from equation (3) by the self-consistency consideration. For comparison the Born values are also evaluated. The results are displayed in table 3. The direct scattering amplitudes obtained by using the above two sets of values of a and b are displayed in table 1 for 100 eV, a typical intermediate energy for both hydrogen and helium. Previous results of Das and associates for the optimal set of values of a and b are also presented in this table as are the first and the second Born amplitudes for the sake of comparison. The results for the differential cross sections are presented in figure 1 for scattering by the hydrogen atom and in figure 2 for scattering by the helium atom. In the figures we have compared our results with those obtained previously by Das and associates which used the least-squares estimates of a and b. In the graphs we have compared our results with other good theoretical results such as those of Scott and Taylor (1979b), Byron and Joachain (1977) for the helium atom and Fon *et al* (1978) and Byron and Joachain (1977) for the hydrogen

Table 1. Comparison of the scattering amplitudes (direct) for the elastic scattering at 100 eV energy.

θ(deg)	FB[a]	SB[b]	O[c]	SC[d]	B[e]
e^-–H					
10	0.9221	1.2243+i0.8836	0.6202+i0.8184	0.9252+i0.5365	0.5384+i0.4767
30	0.5595	0.6486+i0.2419	0.4815+i0.2277	0.5638+i0.1481	0.4567+i0.1341
60	0.2383	0.2870+i0.1344	0.1943+i0.1261	0.2402+i0.0821	0.1808+i0.0740
90	0.1298	0.1589+i0.1012	0.0912+i0.0905	0.1272+i0.0604	0.0839+i0.0515
120	0.0886	0.1090+i0.0821	0.0549+i0.0715	0.0847+i0.0484	0.0502+i0.0400
140	0.0757	0.0932+i0.0749	0.0443+i0.0646	0.0715+i0.0440	0.0403+i0.0359
e^-–He					
10	0.7637	1.4415+i0.8322	0.6675+i1.029	0.9211+i0.3959	−0.1386+i0.1770
30	0.5950	0.8510+i0.4372	0.5466+i0.4542	0.6398+i0.1960	0.1613+i0.0173
60	0.3488	0.4962+i0.2278	0.3285+i0.2487	0.3774+i0.1038	0.1172+i0.0196
90	0.2199	0.3332+i0.1833	0.1743+i0.1955	0.2410+i0.0829	0.0356+i0.0118
120	0.1595	0.2514+i0.1635	0.1008+i0.1666	0.1748+i0.0729	−0.0011+i0.0036
140	0.1389	0.2222+i0.1559	0.0761+i0.1548	0.1518+i0.0689	−0.0126+i0.0002

[a] First Born approximation.
[b] Second Born approximation.
[c] Results with optimal values of a and b.
[d] Results with self-consistent values of a and b.
[e] Results using Born values for a and b.

atom. The comparison shows good agreement of the present set of results with those of other elaborate calculations and with the experimental sets in general. At lower energies, say 30 eV for hydrogen and 50 eV for helium, the cross sections with the exchange amplitude calculated by the Ochkur approximation produce an overestimate, except at small angles, whereas the corresponding results with the exchange amplitude calculated using the Ochkur–Das approximation agree well with the experimental values.

On the whole, at higher energies, the cross sections calculated with the exchange amplitudes taken in the two alternative ways, agree among themselves as well as with the experimental results (except possibly at very small angles (see figures 1 and 2) where the calculated cross sections are underestimates). It is noteworthy that the behaviour of our results at small angles is the same as those obtained with other good theories.

We have computed the total cross sections for the case in which the Ochkur–Das approximation is used for the exchange amplitude. The results are displayed in table 2. In this table we have compared our results with other theoretical results such as those of Winters *et al* (1974), Vanderpoorten (1975), Das *et al* (1980), Fon *et al* (1978) and the EBS theory of Byron and Joachain (1977) for the hydrogen atom and of Dewangan and Walters (1977), Scott and Taylor (1979) and the optical-model theory of Byron and Joachain (1977) for the helium atom. The same table shows experimental results for both hydrogen and helium atoms. The comparison shows a good agreement of the present sets of results with those of other elaborate calculations and of the experimental sets in general.

Next, let us scrutinise our present calculation more thoroughly in the light of previous calculations. First we note from table 3 that the self-consistent values of a agree reasonably well with the optimal values. However, at smaller energies the

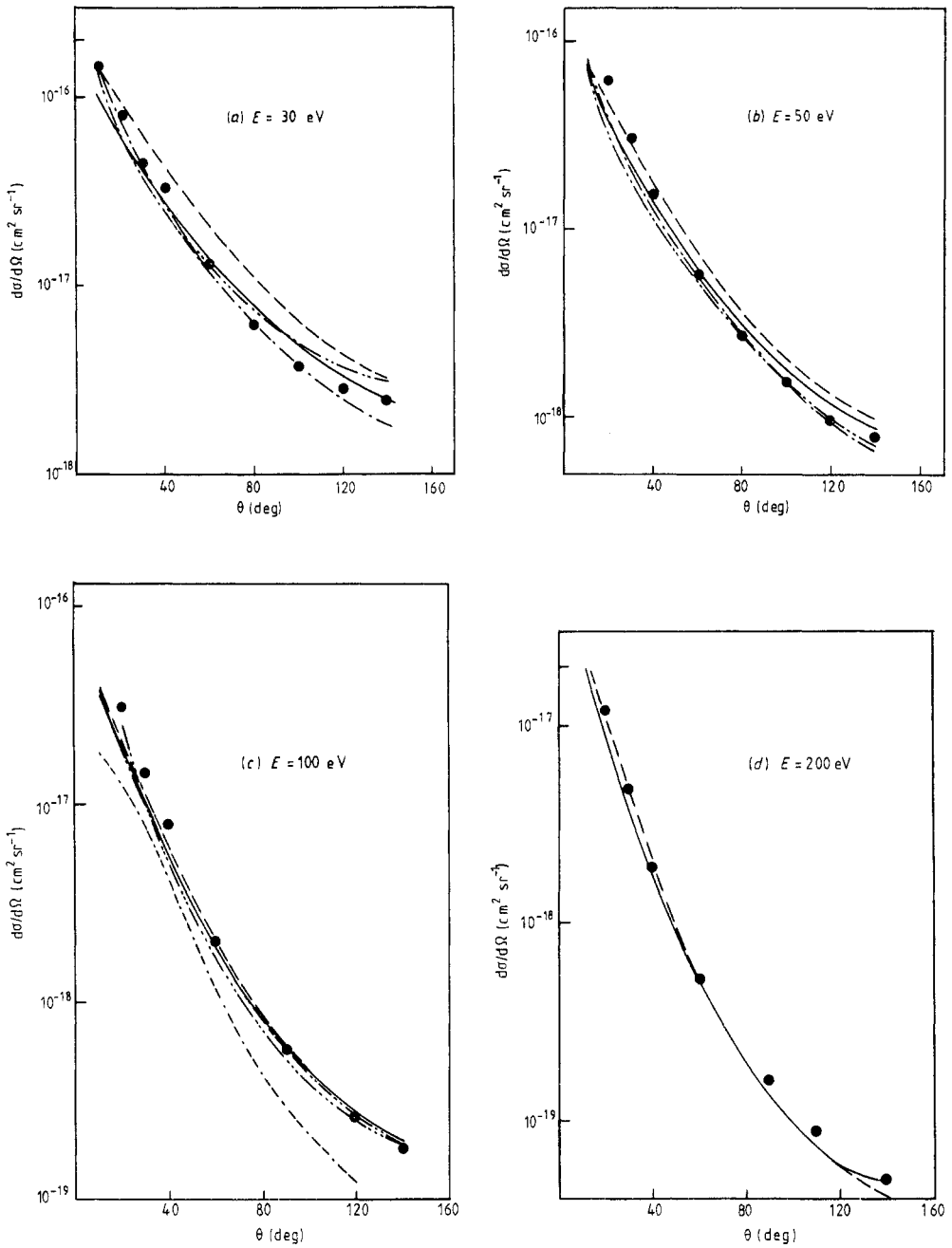

Figure 1. Differential cross sections for the elastic electron–hydrogen scattering at energies (*a*) 30, (*b*) 50, (*c*) 100 and (*d*) 200 eV. Theoretical curves: ———, present calculation with self-consistent *a*, *b* and Ochkur–Das approximation exchange; – – – –, present calculation with self-consistent *a*, *b* and Ochkur approximation exchange; – – · – –, present calculation with Born *a*, *b* and Ochkur–Das approximation exchange; – · – · –, Das and Biswas (1980); – ··· –, Fon *et al* (1978); – ···· –, Byron and Joachain (1977). Experimental values: ●, Williams (1975).

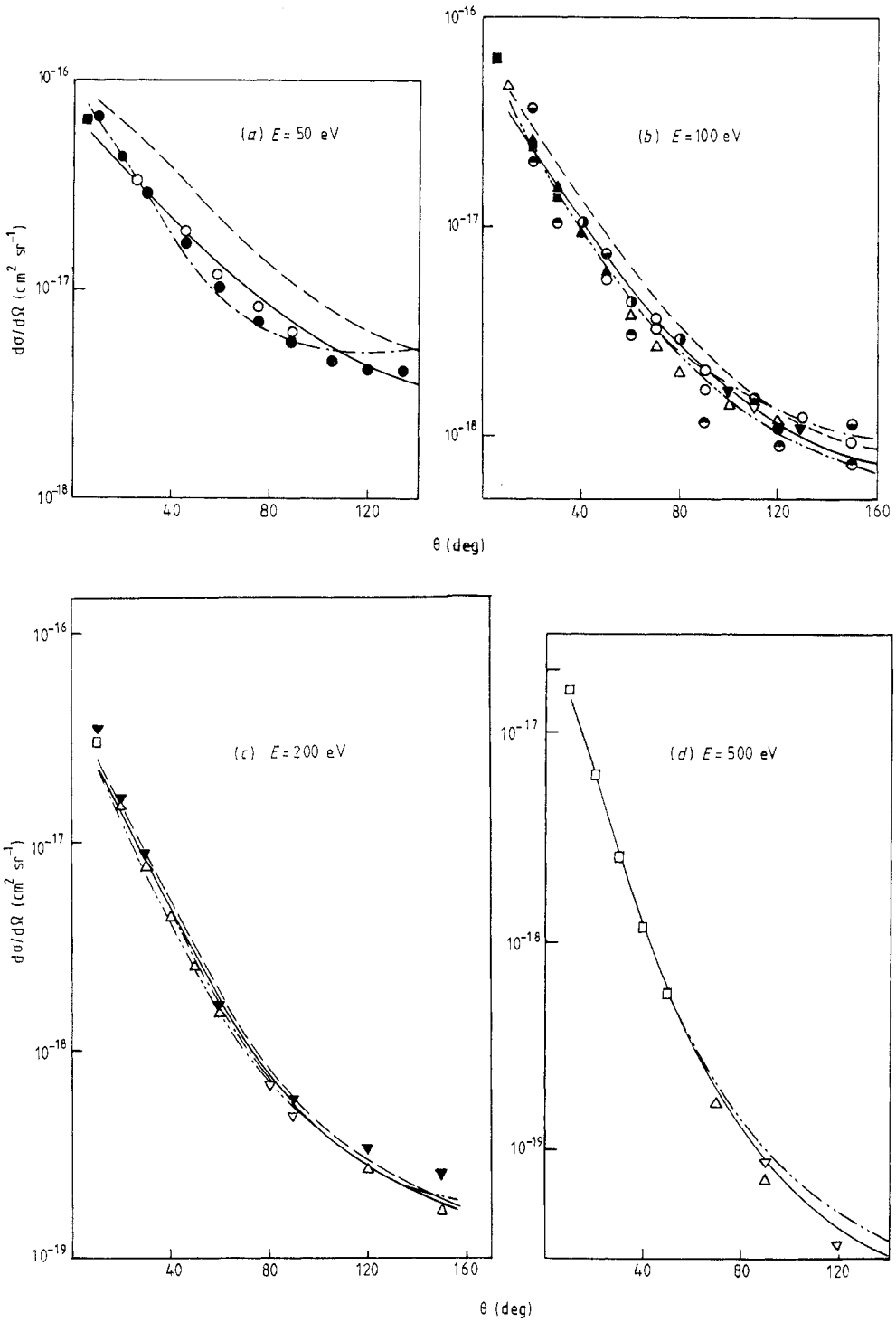

Figure 2. Differential cross sections for the elastic electron–helium scattering at energies (*a*) 50, (*b*) 100, (*c*) 200 and (*d*) 500 eV. Theoretical curves: ———, present calculation with self-consistent *a*, *b* and Ochkur–Das approximation exchange; – – – –, present calculation

Table 2. Total cross sections for elastic scattering in units of a_0^2.

Electron energy (eV)	e^-–H (theory)							e^-–H (experiment)
	a	b	c	d	e	f	g	h
50	1.77	3.24	3.08	4.37	2.71	2.81	2.99	3.62
100	0.939	1.40	1.31	1.57	1.27	1.31	1.24	1.76
200	0.484	0.581	0.581	0.634	0.565	0.542	0.548	0.862

Electron energy (eV)	e^-–He (theory)								e^-–He (experiment)
	a	b	i	j	d	k	f	g	l
100	1.29	2.37	2.38	2.52	2.41	2.05	2.03	2.02	2.04
200	0.691	0.999	1.00	1.04	1.04	0.917	0.889	0.92	0.930
500	0.292	0.336	0.346	0.342	0.351	—	0.324	0.318	0.300

[a] First Born approximation.
[b] Winters *et al* (1974).
[c] Vanderpoorten (1975).
[d] EBS theory of Byron and Joachain (1977).
[e] Fon *et al* (1978).
[f] Das *et al* (1980).
[g] Present calculation with Ochkur–Das exchange approximation.
[h] Williams (1975).
[i] Dewangan and Walters (1977).
[j] Optical-model theory of Byron and Joachain (1977).
[k] Scott and Taylor (1979a, b).
[l] Register *et al* (1979) results quoted in Scott and Taylor (1979a, b).

Table 3. Values of parameters a and b.

E (eV)	Optimal value		Self-consistent value		Born value	
	a	b	a	b	a	b
e^-–H						
30	0.289	0.805	0.405	0.110	−0.301	0.624
50	0.526	0.733	0.465	0.140	0.037	0.607
100	0.725	0.589	0.546	0.183	0.350	0.554
200	0.845	0.452	0.623	0.208	0.556	0.481
400	0.919	0.333	0.699	0.216	0.693	0.404
e^-–He						
50	0.132	1.051	0.302	0.073	−1.13	0.756
100	0.533	0.863	0.379	0.119	−0.403	0.756
200	0.715	0.663	0.455	0.166	0.061	0.706
500	0.853	0.459	0.558	0.212	0.435	0.595

Figure 2—continued.
with self-consistent a, b and Ochkur approximation exchange; –·–·–, Scott and Taylor (1979b); –··–, Das *et al* (1981). Experimental values: ●, Register *et al* (1979) quoted by Scott and Taylor (1979a, b); ■, Chamberlain *et al* (1970); ▲, Jansen *et al* (1976); ▼, Kurepa and Vuskovic (1975); ◒, Crooks and Rudd (1972); ◓, Hughes *et al* (1932); ○, McConkey and Preston (1975); □, Bromberg (1969, 1974); △, Sethuraman *et al* (1974); ▽, Oda *et al* (1972); ◑, Williams (1969).

self-consistent values of b are somewhat too small. This does not affect the values of the scattering amplitudes too much. The reasons for the differences which are observed in the self-consistent and the optimal values are several. Firstly, the asymptotic values of a and b, even if obtained from equation (3) exactly, may not agree with the optimal values too closely. If they did agree it would be a very interesting situation. Secondly, the *exact* values cannot be obtained from equation (3). Only an approximate set of values may be obtained by replacing T_{00} in this equation by some approximate value, so additional differences are introduced by replacing the exact T_{00} by the corresponding asymptotic value. Thus the differences which are observed in the values of a and b in the self-consistent calculation compared with the optimal set are not too serious in view of the above considerations. The reasonable agreement of the results using the self-consistent values with those using optimal values is very encouraging. Use of the Born approximation in equation (3) gives still worse results for scattering amplitudes and the differential cross sections. These may be observed from table 1 and figure 1. However, in this approximation the values of b which are obtained agree with the optimal values. The reason for this may be that the Born amplitude T_{00}^{B} gives a good approximation for the real part of the on-shell elastic scattering amplitude T_{00} (see table 1) which is the main contributor to the values of b. In spite of this good agreement in the values of b with those of its optimal values, the computed scattering amplitudes and the differential cross sections are not good enough. This is primarily because the values of a here determine the accuracy of the cross sections. In any case the reasonable agreement between the results using the self-consistent values of a and b, and those using the optimal values of a and b, permits sufficient confidence to be placed in the calculational method of Das.

4. Conclusions

Our primary aim of this article was to see how closely the values of a and b, determined by equation (3) agreed with the optimal values obtained by the least-squares method and also to examine the accuracy of the resulting differential cross sections. The set of values of a and b obtained in one of the approximations, namely the self-consistency approximation, gives differential cross sections sufficiently accurately. However, the agreement in the values of a and b themselves, obtained in this way, with the optimal set of values is not too good and the same is true for the scattering amplitudes.

In the computational scheme of Das unitarity is not guaranteed except at very high energies for which $\operatorname{Im} f^{(\mathrm{out})}(0) \to f_{\mathrm{B_2I}}(0)$ and

$$f_{n0}^{(\mathrm{out})}(\boldsymbol{k}_n, \boldsymbol{k}_i; \varepsilon_n, \varepsilon_i) \sim f_{n0}^{\mathrm{B}}(\boldsymbol{k}_n, \boldsymbol{k}_i; \varepsilon_n, \varepsilon_i).$$

However it might be possible to incorporate approximately the unitarity condition in the computational scheme. In a coupled scheme of computation for 1S–1S, 1S–2S, 1S–2p transitions in electron–hydrogen scattering, which is in progress, attempts will be made to satisfy the unitarity condition.

Acknowledgments

One of the authors (N Saha) is grateful to the University Grants Commission for awarding a research fellowship.

References

Bromberg J P 1969 *J. Chem. Phys.* **50** 3906
—— 1974 *J. Chem. Phys.* **61** 963
Buckley B D and Walters H R J 1974 *J. Phys. B: At. Mol. Phys.* **7** 1380
Byron F W Jr and Joachain C J 1973 *Phys. Rev.* A **8** 1267 and 3266
—— 1977 *J. Phys. B: At. Mol. Phys.* **10** 207
Chamberlain G E, Mielczarek S R and Kuyatt C E 1970 *Phys. Rev.* A **2** 1905
Crooks G B and Rudd M E 1972 *Bull. Am. Phys. Soc.* **17** 131
Das J N 1979 *Phys. Lett.* **69A** 405
Das J N, Bera R K and Patra B N 1981 *Phys. Rev.* A **23** 732
Das J N and Biswas A K 1980 *Phys. Lett.* **78A** 319
—— 1981 *J. Phys. B: At. Mol. Phys.* to be published
Dewangan D P and Walters H R J 1977 *J. Phys. B: At. Mol. Phys.* **10** 637
Fon W C, Burke P G and Kingston A E 1978 *J. Phys. B: At. Mol. Phys.* **11** 521
Hughes A L, McMillen J H and Webb G M 1932 *Phys. Rev.* **41** 154
Jansen R H J, de Heer F J, Luyken H J, van Wingerden B and Blaauw H J 1976 *J. Phys. B: At. Mol. Phys.* **9** 185
Kurepa M V and Vuskovic L D 1975 *J. Phys. B: At. Mol. Phys.* **8** 2067
McConkey J W and Preston J A 1975 *J. Phys. B: At. Mol. Phys.* **8** 63
Oda N, Nishimura F and Tihara S 1972 *J. Phys. Soc. Japan* **33** 467
Register D, Trajmar S and Srivastava S K 1979 to be published
Saha N 1980 unpublished
Scott T and Taylor H S 1979a *J. Phys. B: At. Mol. Phys.* **12** 3367
—— 1979b *J. Phys. B: At. Mol. Phys.* **12** 3385
Sethuraman S K, Rees J A and Gibson J R 1974 *J. Phys. B: At. Mol. Phys.* **7** 1741
Vanderpoorten R 1975 *J. Phys. B: At. Mol. Phys.* **8** 926
Williams J F 1975 *J. Phys. B: At. Mol. Phys.* **8** 2191
Williams K G 1969 *Proc. 6th Int. Conf. on Physics of Electronic and Atomic Collisions* (Massachussets: MIT Press) p 735
Winters K H, Clark C D, Bransden B H and Coleman J P 1974 *J. Phys. B: At. Mol. Phys.* **7** 788