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The elastic scattering of electrons from inert gases I. Helium

W C Font†, K A Berrington and A Hibbert

Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast, Belfast BT7 1NN, Northern Ireland

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Abstract. The R-matrix calculations of O'Malley *et al* are simplified and extended to the intermediate impact energy range in which the He ground-state wavefunction is coupled with a ^{1}P pseudo-state to include the full static dipole polarisability. Phaseshifts, differential, integrated and momentum transfer cross sections for electrons elastically scattered from helium are reported for the impact energy range of 5 to 200 eV. At low energies the present calculation essentially reproduces the results of O'Malley *et al* for $5 \leq E \leq 16{\cdot}5$ eV. At intermediate energies good agreement between the present calculations and the most recent measurements is observed.

1. Introduction

This paper is the first of a series which studies the phaseshifts, differential and momentum transfer cross sections of electrons elastically scattered from inert-gas atoms by using the R-matrix method in which the ground-state wavefunction is coupled only with a ^{1}P pseudo-state to allow for the full static dipole polarisability.

In recent years there has been renewed interest and intensive experimental efforts devoted to the study of elastic scattering of electrons by atoms because most data were considered to be not of sufficient accuracy and were only available in a limited energy and angular range. In general, most data available are only relative measurements which is due to the difficulty of calibration in scattering experiments (Moiseiwitsch and Smith 1968). It would be very useful if some easily measurable electron scattering cross sections were accurately known so that it could be used as a standard against which all future cross section measurements could be calibrated. There are also new developments in the experimental and theoretical investigation of the spin polarisation of electrons following elastic scattering from atoms. In the past, this has mainly centred on heavy atoms and at high energy. Recent studies show that significant polarisation can be observed at much lower electron impact energy and for much lighter atoms. As discussed by Bühring (1968) total polarisation occurs at electron energies and scattering angles close to the electron energy where a cross section minimum has its smallest value (the critical energy and critical angle). Because of their relatively simple structure, inert gases have been the subject of extensive investigations, experimentally and theoretically.

The aims of this series of papers are as follows: (i) to provide a simple calculation capable of high accuracy over a large energy range, covering the low impact energy

† Commonwealth Fellow on sabbatical leave from the Department of Mathematics, University of Malaya, Kuala Lumpur, Malaysia.

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region and up into the region of intermediate energy to serve as a future standard; and (ii) to develop a method which can be extended to other heavier atomic systems, in particular the inert gases, in order to provide useful information in the search of critical energy where large spin polarisation might be observed.

Among all the inert gases, elastic electron–helium scattering stands out as the ideal candidate to serve as standard. Experimentally, helium is one of the easiest gases to work with and detailed experimental data are available (see Bransden and McDowell 1978). Theoretically, highly accurate calculations are available over a large energy range below the first excitation threshold (O'Malley *et al* 1979, Nesbet 1979). However, it would be difficult to extend these calculations in their existing form to energies well beyond the first excitation threshold. For the last ten years the extended polarised-orbital calculation of LaBahn and Callaway (1970) seems to be the only calculation which provides reasonable agreement with experiments from low energies to intermediate energies. At high energies the eikonal Born series of Byron and Joachain (1977b) might be accurate. Register *et al* (1980) recently reported absolute differential, integral and momentum transfer cross sections for electrons elastically scattered from helium for the impact energy range of 5 to 200 eV. It would be useful to provide an accurate calculation to compare with their measurements.

2. *R*-matrix calculation

In this paper we simplify the calculations of O'Malley *et al* (1979) in the following ways. (i) The 1^1S He ground state and the ^{1}P pseudo-state are formed only by the Hartree–Fock 1s orbital plus five pseudo-orbitals from 2s to 3d to allow only for the full static dipole polarisability of the ground state. (ii) We adopt the conventional published version of the *R*-matrix method (Berrington *et al* 1978).

The pseudo-orbitals included are simultaneously optimised to minimise the ground-state energy and maximise the dipole polarisability as described by O'Malley *et al* (1979). The quadrupole polarisability is neglected through the exclusion of the ^{1}D pseudo-state. The quadrupole and higher multipoles are thought to be important only for near zero-energy electron scattering with helium and are not expected to make a significant contribution to the energy range in question. As will be shown in § 3, the present calculation reproduces the results of O'Malley *et al* (1979) over the energy range $5 \leqslant E \leqslant 16{\cdot}5$ eV and this agreement fully justifies the exclusion of higher poles other than dipole in the ground-state polarisability.

In this paper we adopt the *R*-matrix radius, $a = 10$ au, and the number of continuum orbitals included for each angular momentum is twenty. The CI wavefunctions for the ground state and ^{1}P pseudo-state give the ground-state energy at $-2{\cdot}89825$ au and the ^{1}P pseudo-threshold at $-1{\cdot}93179$ au. The static dipole polarisability obtained by coupling the 1^1S ground state to the ^{1}P pseudo-state is not significantly different from that calculated by O'Malley *et al* (1979). In the present calculation only partial waves up to $L = 13$ are calculated directly by the *R*-matrix program: for $L \geqslant 14$ and for $E \leqslant 80$ eV the *T*-matrix elements converge well to those obtained by

$$T_L = 2(\tan \delta_L)^2 - 2\mathrm{i} \tan \delta_L \tag{1}$$

where

$$\tan \delta_L = \frac{\pi \alpha k^2}{(2L+3)(2L+1)(2L-1)} \tag{2}$$

while α is the dipole polarisability. At higher energies, a few more partial waves ($L \geq 14$) are extrapolated to give smooth convergence to the T-matrix elements obtained by equation (1), through the effective range formula of Rosenberg *et al* (1961). The highest partial wave included is $L = 250$ at 200 eV.

One difficulty of theoretical methods based on a close-coupling expansion, such as the R-matrix method, arises from the inclusion of three-electron correlation terms in the expansion of the total wavefunction (see Fon *et al* 1979). These terms are included for completeness and in addition they allow for important correlation effects at low energies when all three electrons are close together near the nucleus. However, in the energy range $E \geq 35$ eV they give rise to pseudo-resonances in the scattering amplitude and cross section. Since the three-electron correlation terms are chosen to simulate the low-lying physical He^- bound states, the pseudo-resonances lie below 150 eV. T-matrix elements for impact energies in this region of pseudo-resonances were extracted by using an averaging technique described in the previous paper (Burke *et al* 1981).

Finally, it is clear that the present calculation will not show the resonance structure in the excited-state threshold region apart from that due to the pseudo-state threshold. The results should therefore be treated with caution in the energy range 19·3 to 27 eV.

3. Results and discussion

We calculate phaseshifts, integral, differential and momentum transfer cross sections for the following process:

$$e + He(1^1S) \rightarrow e + He(1^1S)$$

at impact energies ranging from 5 to 200 eV. The present calculations are given in tables 1–7, and figures 1–6 where comparison of the present calculation and other theoretical calculations and experimental measurements is also made.

3.1. Phaseshifts for S, P and D partial waves

At low impact energies, electron scattering from ground-state helium can be characterised by a few of the lowest partial waves from which integral, momentum transfer and differential cross sections can be calculated. Among others, the variational calculations of Sinfailam and Nesbet (1972), Nesbet (1979) and the R-matrix calculation of O'Malley *et al* (1979) are considered to be the most ambitious *ab initio* calculations. In table 1, the present R-matrix calculation is compared with these calculations. It is noted that present calculations are not significantly different from those of O'Malley *et al* (1979) over the energy range $5 \leq E \leq 16{\cdot}5$ eV. Good agreement is observed between the present calculation and those of Sinfailam and Nesbet (1972) and Nesbet (1979).

For the comparison of measured and computed data, the experimental result has to be brought to a suitable scale. A phaseshift analysis of the experimental data in He consistent with the forward dispersion relation has been performed and discussed (Gerjuoy and Krall 1960, 1962, Bransden and McDowell 1969, Nacache and McDowell 1974, Bransden and Hutt 1975). However, it has become clear (Byron *et al* 1975, Blum and Burke 1976, Hutt *et al* 1976) that the forward dispersion relation does not hold in general for electron–atom scattering. Specifically, it does not hold in the e^-–He case. Greater emphasis must be placed on an accurate experimental determination of the first few phaseshifts. This can be done by making absolute differential

Table 1. The elastic scattering phaseshifts δ_L for the electron–helium system.

	δ_0				δ_1				δ_2			
k_0^2 (Ryd)	(*a*)	(*b*)	(*c*)	(*d*)	(*a*)	(*b*)	(*c*)	(*d*)	(*a*)	(*b*)	(*c*)	(*d*)
0·36	2·3463	2·349	2·3486	2·3638	0·116	0·116	0·1209	0·120	0·0142	—	0·0149	0·141
0·49	2·2309	—	2·2349	2·2518	0·1524	—	0·1588	0·1567	0·0193	—	0·0203	0·0197
0·64	2·1234	2·124	2·1261	2·1338	0·1883	0·189	0·1960	0·1949	0·0253	—	0·0265	0·0258
0·81	2·0244	2·028	2·0253	2·0428	0·2221	0·224	0·2305	0·2311	0·0320	—	0·0335	0·0322
1·00	1·9339	—	1·9359	1·9550	0·2528	—	0·2626	0·2646	0·0396	—	0·0414	0·0393
1·21	1·8516	1·853	1·8568	1·8765	0·2796	0·281	0·2932	0·2927	0·0482	—	0·0501	0·0473

(*a*) Present *R*-matrix calculation.
(*b*) *R*-matrix calculation of O'Malley *et al* (1979).
(*c*) Nesbet (1979).
(*d*) Sinfailam and Nesbet (1972).

cross section measurements and then performing a phaseshift analysis of the measurements. Among others, Andrick and Bitsch (1975) and Williams (1979) have performed phaseshift analyses of their experimental angular distributions of electrons elastically scattered from ground-state He and have obtained s, p and d phaseshifts. In table 2, the present calculation is compared with those experimental phaseshifts derived by Williams. Excellent agreement is observed between the present calculation and the measurements. Other calculations on low-energy phaseshifts include the earlier polarised-orbital calculations of Callaway *et al* (1968), LaBahn and Callaway (1970), Duxler *et al* (1971) and recently Yau *et al* (1978); the many-body theory of Knowles and McDowell (1973), Yarlagadda *et al* (1973); the close-coupling calculations of Burke *et al* (1969) and Burke and Robb (1972) and the variational calculations of Wichmann and Heiss (1974). Recent reviews have been given by Moiseiwitsch (1977), Burke and Williams (1977) and Steph *et al* (1979).

Table 2. The elastic scattering phaseshifts δ_L for the electron–helium system.

	δ_0		δ_1		δ_2	
E(eV)	(*a*)	(*b*)	(*a*)	(*b*)	(*a*)	(*b*)
4·91	2·332	2·3454	0·127	0·1163	0·0132	0·0143
5·02	2·322	2·3375	0·129	0·1187	0·0136	0·0146
5·51	2·283	2·3034	0·140	0·1291	0·0152	0·0160
6·10	2·242	2·2651	0·152	0·1412	0·0172	0·0176
6·66	2·207	2·2313	0·161	0·1522	0·0188	0·0192
7·01	2·181	2·2111	0·168	0·1589	0·0198	0·0203
8·00	2·134	2·1580	0·186	0·1766	0·0228	0·0232
8·71	2·098	2·1233	0·196	0·1884	0·0251	0·0253
10·00	2·036	2·0656	0·216	0·2080	0·0302	0·0290
11·00	2·003	2·0252	0·229	0·2219	0·0334	0·0319
12·00	1·968	1·9880	0·242	0·2346	0·0372	0·0348
13·00	1·936	1·9536	0·254	0·2463	0·0406	0·0378
14·00	1·908	1·9215	0·267	0·2569	0·0444	0·0408
15·00	1·881	1·8917	0·278	0·2667	0·0471	0·0438
16·00	1·857	1·8638	0·289	0·2756	0·0501	0·0468
17·00	1·833	1·8378	0·298	0·2840	0·0527	0·0498
18·00	1·815	1·8135	0·305	0·2917	0·0556	0·0526
19·00	1·800	1·7907	0·311	0·2990	0·0580	0·0555

(*a*) Experimental measurements of Williams (1979).
(*b*) Present R-matrix calculation.

3.2. *Differential elastic cross sections*

At impact energies above the inelastic threshold, the phaseshift analysis discussed in § 3.1 on experimental data is no longer appropriate. The presence of open inelastic and ionisation channels introduces absorptive terms in the effective scattering potential which facilitate the loss of flux through these channels. In general, it is the direct measurement of differential cross sections rather than the derived experimental phaseshifts which provides the most sensitive and direct comparison with theoretical calculations.

The present differential cross sections are summarised in tables 3 and 4 and some of the results are shown and compared with other theoretical calculations and experimental measurements in figures 1–6.

The earlier differential cross section measurements (Ramsauer and Kollath 1932, Bullard and Massey 1931, Mehr 1967) show only qualitative agreement between each other and are not consistent with modern theoretical work. We shall exclude them from our later discussion. Although considerable experimental measurements have been performed recently at impact energies of 100 and 200 eV, relatively few experiments have been made at energies less than 100 eV.

In figure 1, the present R-matrix calculation is shown at 5 eV. There is good agreement between the present calculation and that of Nesbet (1979) and both are consistent with the measurements of Andrick and Bitsch (1975) and Register *et al* (1980). However, the polarised-orbital calculation underestimates the cross section at small scattering angles. The measurements of McConkey and Preston (1975) and Gibson and Dolder (1969a, b) deviate qualitatively and quantitatively from the experiments and calculations mentioned above. In figure 2, the present R-matrix calculation at 12 and 19 eV is shown. There is good agreement between the present calculation and those of Nesbet (1979) and LaBahn and Callaway (1970) and with the measurements of Andrick and Bitsch (1975) and Register *et al* (1980). Again the shape of the measurement of McConkey and Preston (1975) seems to deviate from the rest.

In the intermediate energy range $30 \leqslant E \leqslant 80$ eV, we would expect the greatest discrepancy between calculations and experimental measurements for the simple reason that there are very few theoretical calculations which are expected to be good in this energy range where all channels are open and inelastic scattering ionisation and

Table 3. Differential cross section for elastic electron–helium scattering (in units of 10^{-17} cm^2 sr^{-1}).

Angle (deg)	Electron energy (eV)						
	5	12	18	19	20	30	40
0	2·408	5·171	6·751	6·941	7·132	8·601	9·430
5	2·391	4·826	6·159	6·315	6·470	7·581	8·147
10	2·388	4·466	5·559	5·680	5·800	6·599	6·903
20	2·419	3·859	4·553	4·620	4·681	4·997	4·890
30	2·510	3·389	3·764	3·790	3·808	3·798	3·455
40	2·662	3·043	3·160	3·155	3·142	2·921	2·477
50	2·871	2·813	2·716	2·687	2·652	2·290	1·830
60	3·136	2·689	2·410	2·361	2·311	1·847	1·408
70	3·449	2·660	2·220	2·155	2·091	1·545	1·136
80	3·801	2·713	2·124	2·045	1·969	1·347	9·630
90	4·181	2·831	2·103	2·010	1·921	1·227	8·563
100	4·575	2·997	2·136	2·029	1·927	1·165	7·944
110	4·970	3·194	2·205	2·083	1·970	1·146	7·620
120	5·320	3·403	2·295	2·158	2·032	1·156	7·480
130	5·701	3·609	2·392	2·240	2·103	1·184	7·440
140	6·009	3·797	2·484	2·320	2·171	1·221	7·442
150	6·262	3·956	2·563	2·389	2·229	1·258	7·452
160	6·449	4·077	2·623	2·442	2·273	1·289	7·456
170	6·564	4·152	2·659	2·475	2·300	1·310	7·456
180	6·601	4·176	2·671	2·486	2·309	1·316	7·457

Table 4. Differential elastic cross sections (10^{-17} cm^2 sr^{-1}).

Angle (deg)	Electron energy (eV) 50	60	80	90	100	150	200
0	9·663	9·391	8·646	8·213	7·819	6·724	6·093
5	8·195	7·801	6·890	6·410	5·998	4·682	3·980
10	6·763	6·263	5·243	4·750	4·360	3·152	2·612
20	4·497	3·924	3·017	2·645	2·372	1·672	1·410
30	2·999	2·513	1·882	1·648	1·479	1·029	8·286^{-1}
40	2·061	1·694	1·262	1·101	9·859^{-1}	6·430^{-1}	4·774^{-1}
50	1·480	1·204	8·943^{-1}	7·764^{-1}	6·885^{-1}	4·089^{-1}	2·774^{-1}
60	1·118	9·050^{-1}	6·613^{-1}	5·671^{-1}	4·970^{-1}	2·676^{-1}	1·654^{-1}
70	8·875^{-1}	7·114^{-1}	5·067^{-1}	4·290^{-1}	3·702^{-1}	1·815^{-1}	1·031^{-1}
80	7·378^{-1}	5·826^{-1}	4·004^{-1}	3·348^{-1}	2·851^{-1}	1·303^{-1}	6·862^{-2}
90	6·388^{-1}	4·936^{-1}	3·243^{-1}	2·676^{-1}	2·255^{-1}	9·868^{-2}	4·915^{-2}
100	5·728^{-1}	4·306^{-1}	2·684^{-1}	2·188^{-1}	1·830^{-1}	7·849^{-2}	3·750^{-2}
110	5·288^{-1}	3·867^{-1}	2·275^{-1}	1·829^{-1}	1·521^{-1}	6·530^{-2}	2·994^{-2}
120	4·999^{-1}	3·577^{-1}	1·990^{-1}	1·576^{-1}	1·301^{-1}	5·559^{-2}	2·450^{-2}
130	4·814^{-1}	3·402^{-1}	1·808^{-1}	1·408^{-1}	1·151^{-1}	4·878^{-2}	2·047^{-2}
140	4·699^{-1}	3·311^{-1}	1·710^{-1}	1·313^{-1}	1·054^{-1}	4·358^{-2}	1·775^{-2}
150	4·634^{-1}	3·280^{-1}	1·672^{-1}	1·268^{-1}	1·001^{-1}	4·001^{-2}	1·611^{-2}
160	4·596^{-1}	3·273^{-1}	1·668^{-1}	1·256^{-1}	9·734^{-2}	3·764^{-2}	1·551^{-2}
170	4·580^{-1}	3·281^{-1}	1·677^{-1}	1·257^{-1}	9·659^{-2}	3·629^{-2}	1·537^{-2}
180	4·578^{-1}	3·290^{-1}	1·680^{-1}	1·265^{-1}	9·606^{-2}	3·611^{-2}	1·532^{-2}

The superscript denotes the power of ten by which the number should be multiplied.

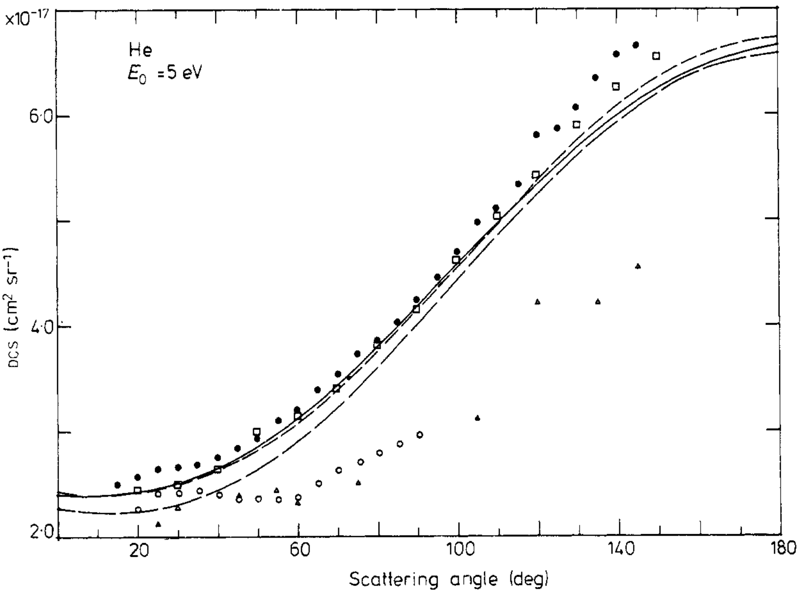


Figure 1. Differential cross sections (10^{-17} cm^2 sr^{-1}) at 5 eV. Experiment: ●, Andrick and Bitsch (1975); ○, McConkey and Preston (1975); □, Register *et al* (1980); △, Gibson and Dolder (1969). Theory: ——, present R-matrix calculation; — —, LaBahn and Callaway (1970); - - -, Nesbet (1979).

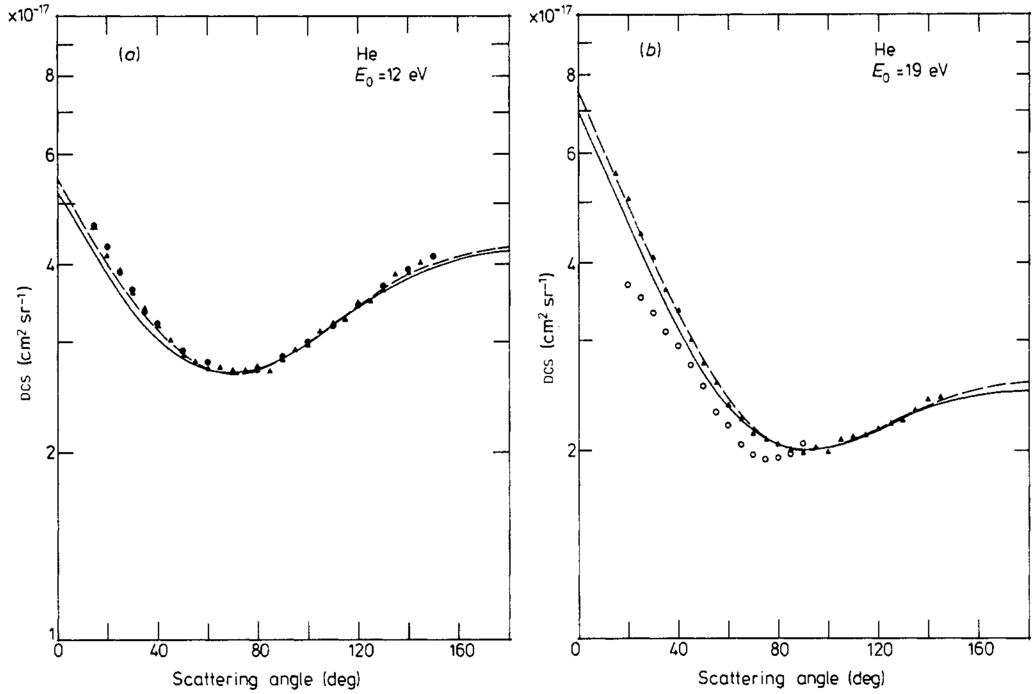
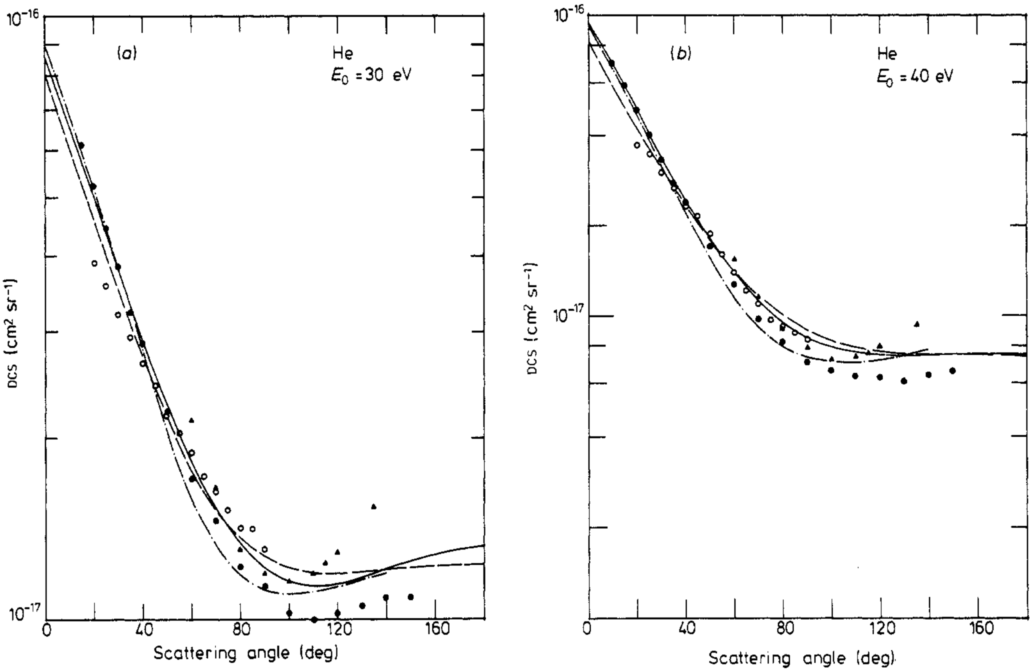


Figure 2. Differential cross sections (10^{-17} cm^2 sr^{-1}) at (*a*) 12 eV, (*b*) 19 eV. Experiment: ●, Register *et al* (1980); ▲, Andrick and Bitsch (1975); ○, McConkey and Preston (1975). Theory: ——, present R-matrix calculation; – – –, Nesbet (1980).

other processes are competing with the elastic scattering process. The impact energy here is not high enough for the high-energy approximation (e.g. eikonal Born series) to hold. The only calculation, other than the recent many-body Green function method of Scott and Taylor (1979), available for comparison with experiments is the polarised-orbital calculation of LaBahn and Callaway (1970). It is essentially a single-channel scattering approximation which may be expected to be good when the impact energy is low. The effect of loss of flux through open channels which is not allowed for in the polarised-orbital model will be particularly pronounced. In figure 3, the present R-matrix result is shown and compared with other theoretical calculations and experimental measurements at 30, 40 and 80 eV. It is obvious that the experimental measurements (McConkey and Preston 1975, Srivastava and Trajmar 1976, Register *et al* 1980) are not consistent in shape or in magnitude. The measurements of McConkey and Preston (1975) and Srivastava and Trajmar (1976) are limited in the range of scattering angles ($20 < \theta < 90°$ for McConkey and Preston and $60 < \theta < 135°$ for Srivastava and Trajmar) and as a result, the behaviour of the cross section at small and large scattering angles cannot be studied properly. The experiment of Register *et al* is the only one which presents measurements at the full range of the scattering angle ($10 < \theta < 150°$). In comparison with the measurements of Register *et al* the present calculation shows excellent agreement with the measurement for electron scattering angles smaller than 50° and lies considerably above the measurement at larger angles. However, the essential qualitative shape of the measurement of Register *et al* is reproduced, while the calculations of LaBahn and Callaway (1970) and those of Scott and Taylor (1979) underestimate the cross section substantially at small scattering



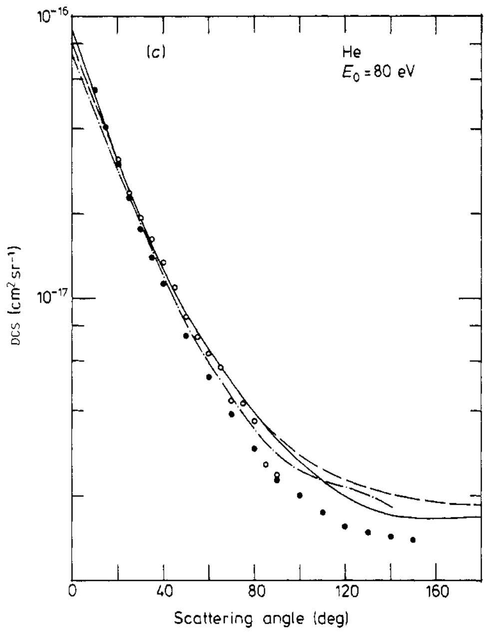


Figure 3. Differential cross sections at (*a*) 30 eV, (*b*) 40 eV, (*c*) 80 eV. Experiment: ●, Register *et al* (1980); ○, McConkey and Preston (1975); △, Srivastava and Trajmar (1976). Theory: ——, present *R*-matrix calculation; — —, LaBahn and Callaway (1970); – · –, Scott and Taylor (1979).

angles (see figure 6 at $\theta_e = 5°$) and the large scattering angle behaviour of Scott and Taylor seems to deviate from the experimental shape.

At 100 and 200 eV impact energies a large number of calculations and measurements have been carried out (figures 4–5). At 100 eV (figure 4(*a*)) the present cross sections are compared with experiments. The data of Jansen *et al* (1976) and Gupta and Rees (1975) agree very well with present calculations. At 200 eV (figure 4(*b*))

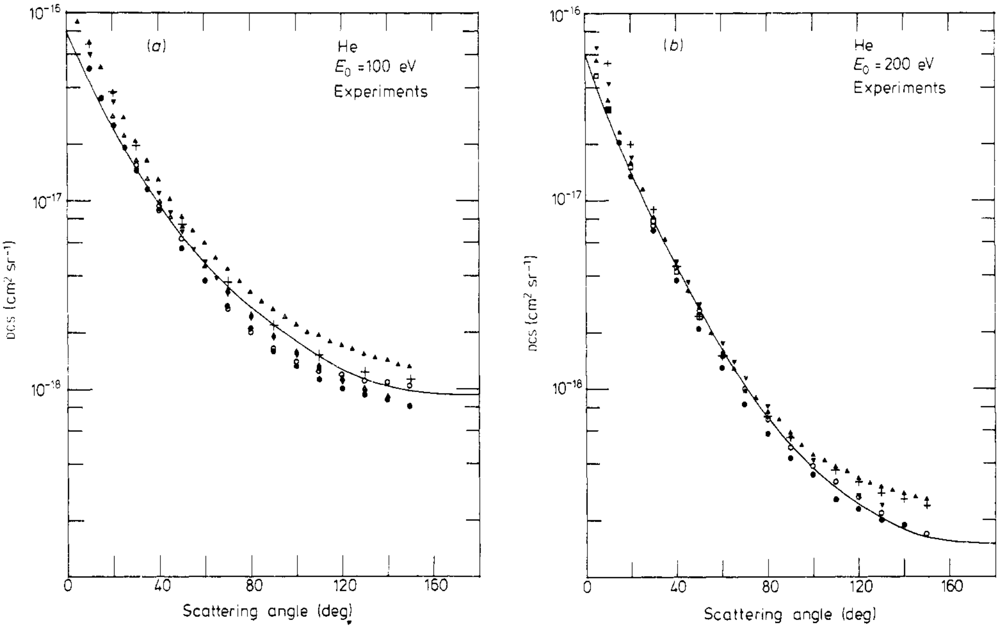


Figure 4. Experimental differential cross sections at (*a*) 100 eV, (*b*) 200 eV. ●, Register *et al* (1980); ○, Sethuraman *et al* (1974); △, Gupta and Rees (1975); ▲, Kurepa and Vušković (1975); +, Crooks and Rudd (1972); □, Jansen *et al* (1976); ▼, Jost *et al* (1973); ——, present R-matrix calculation.

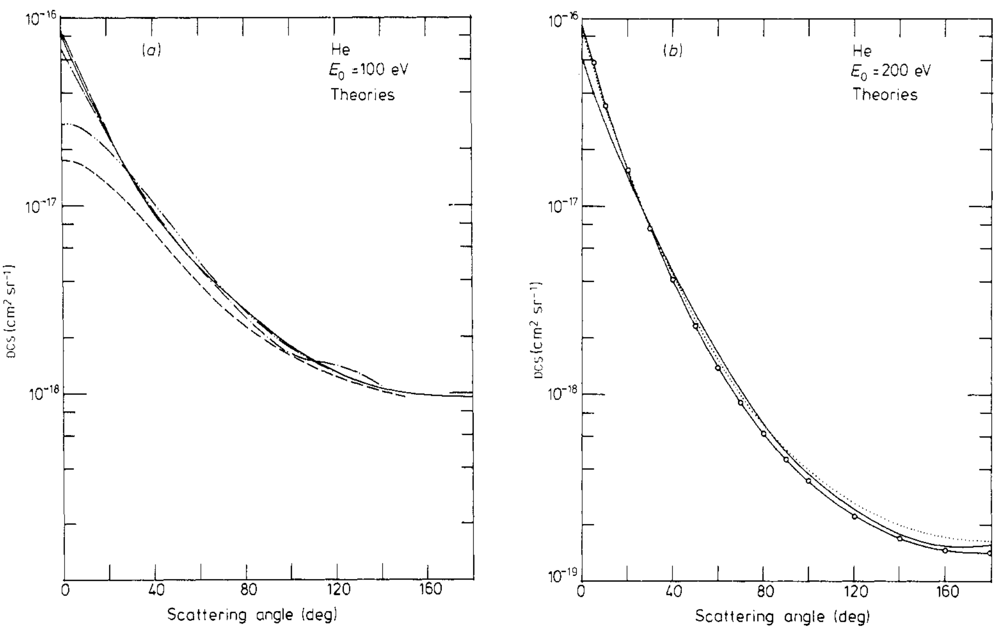


Figure 5. Theoretical differential cross sections at (*a*) 100 eV, (*b*) 200 eV. ——, present R-matrix calculation; — —, LaBahn and Callaway (1970); – · –, Scott and Taylor (1979); – · · · –, Walker (1971); – – –, Fink and Yates (1970); —○—○—, Winters *et al* (1974); · · · · · ·, Byron and Joachain (1977).

comparisons are made of the present results and experimental measurements. The data of Register *et al* (1980), Sethuraman *et al* (1974) and Bromberg (1974) (not shown) seem to give the best agreement with the present calculations. Among the theoretical calculations, at 100 eV (figure 5(*a*)) there is overall agreement between the present calculations and those of LaBahn and Callaway (1970) and Scott and Taylor (1979) except at large scattering angles where the formation of a bump in the calculation of Scott and Taylor needs further explanation. At 200 eV (figure 5(*b*)) the present R-matrix calculation is shown to give excellent agreement with the optical model calculation of Byron and Joachain (1977a) and the second-order potential calculations of Winters *et al* (1974). The latter are the adopted values by Bransden and McDowell (1978). In figure 6, the 5° DCS is compared with the experimental measurements of Register *et al* (1980). While the calculations of LaBahn and Callaway (1970) and Scott and Taylor (1979) are substantially below the experimental measurement from 30 to 100 eV, the present calculations seem to lie within the error bars of Register *et al* (1980). Any suggestion of structure at 20 and 70 eV impact energies is not obvious in our present calculation.

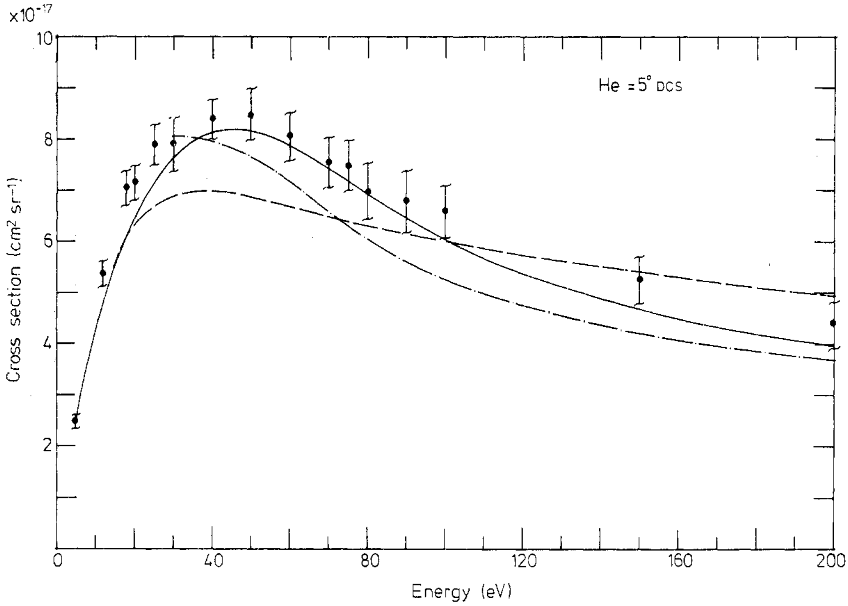


Figure 6. Energy dependence of the 5° differential cross section. ⧫, Register *et al* (1980); ——, present R-matrix calculation; —·—, Scott and Taylor (1979); - - -, LaBahn and Callaway (1970).

Although the Born effective range theory (ERT) of Rosenberg *et al* (1961) written in equation (2) is well known for approximating phaseshifts for large angular momentum at low impact enrgies, it is not clear that the Born ERT can be used for approximating T-matrix elements for high L at impact energies greater than the first excitation threshold. Roughly speaking, at intermediate impact energies and at 'sufficiently' high angular momentum, the incident electrons do not penetrate the inner part of the atom and thus only feel the longest range part of the electron–atom interaction. This is the static dipole polarisation potential. As long as the T-matrix elements are small and the angular momentum is 'sufficiently' high, the Born ERT is expected to be good. However, it is not clear that the highest angular momentum considered by LaBahn and Callaway ($L = 10$) and Scott and Taylor ($L = 8$) in their respective models are 'sufficiently' high for the Born ERT to hold. As the small-angle scattering is essentially dominated by high partial waves, unsatisfactory treatment of high partial waves can cause underestimation of the cross section at a small scattering angle, while the other source of error can come from the very formalism of all single-channel scattering models in which the loss of flux is not allowed for. The loss of flux through open channels is particularly serious at intermediate impact energies.

3.3. Integral elastic and momentum transfer cross sections

Recently several new measurements on total, integral elastic (Kennerly and Bonham 1978, Stein *et al* 1978, Register *et al* 1980) and momentum transfer cross sections (Register *et al*) have been reported. It is interesting to compare our results with these

Table 5. Low-energy integrated elastic cross sections (10^{-16} cm^2).

E(eV)	(*a*)	(*b*)	(*c*)	(*d*)	(*e*)	(*f*)	(*g*)
5·0	5·25	—	5·482	5·365	5·379	5·180	5·640
5·4	—	5·30	—	5·273	5·287	—	—
6·0	5·04	—	—	5·138	5·152	4·987	—
6·4	—	5·09	—	5·051	5·066	—	—
7·0	4·83	—	—	4·923	4·942	4·799	—
7·4	—	4·96	—	4·841	4·864	—	—
8·0	4·64	—	—	4·720	4·749	4·617	—
8·4	—	4·73	—	4·642	4·675	—	—
9·0	4·46	—	—	4·527	4·566	4·444	—
9·4	—	4·54	—	4·453	4·495	—	—
10·0	4·30	—	—	4·345	4·390	4·278	—
10·4	—	4·25	—	4·275	4·322	—	—
11·4	—	4·26	—	4·108	4·155	—	—
12·0	3·96	—	4·127	4·010	4·059	—	4·150
12·4	—	3·94	—	3·949	3·996	—	—
13·4	—	3·92	—	3·799	3·848	—	—
14·0	3·69	—	—	3·713	3·763	—	—
14·4	—	3·64	—	3·657	3·709	—	—
15·0	—	—	—	3·576	—	3·545	—
15·4	—	3·58	—	3·524	3·580	—	—
16·0	3·43	—	—	3·448	3·506	—	—
16·4	—	3·41	—	3·398	3·458	—	—
17·4	—	3·27	—	3·279	3·341	—	—
18·0	3·22	—	3·347	3·212	3·274	—	3·313
18·4	—	3·20	—	3·168	3·230	—	—

(*a*) Experiment, Kennerly and Bonham (1978).
(*b*) Experiment, Stein *et al* (1979).
(*c*) Experiment, Register *et al* (1980).
(*d*) R-matrix calculation (present).
(*e*) Nesbet (1979).
(*f*) LaBahn and Callaway (1970).
(*g*) Experiment, Andrick and Bitsch (1975).

measurements particularly in the energy range $30 \leq E \leq 100$ eV where measurements on these cross sections are lacking.

The present calculations are displayed in tables 5 to 7. Integral cross sections at low impact energies are compared (table 5) with the calculations of Nesbet (1979) and LaBahn and Callaway (1970) and the measurements of Kennerly and Bonham (1978), Stein *et al* (1978) and Register *et al* (1980). Excellent agreement is observed between all the calculations and experimental measurements. In particular, discrepancy among the present calculation, the calculation of Nesbet and the measurement of Stein *et al* (1979) and that of Kennerly and Bonham does not exceed 2%. Similarly, there is a good agreement between the present calculation, the calculation of Nesbet (1979) and

Table 6. Low-energy mom entum transfer cross sections (10^{-16} cm^2).

E(eV)	Register *et al* (1979)	Andrick and Bitsch (1975)	Milloy and Crompton (1977)	Nesbet (1979)	R-matrix calculation (present)
5	6·451	6·64	6·31	6·320	6·278
6	—	—	6·00	5·994	5·959
7	—	—	5·68	5·670	5·633
8	—	—	5·35	5·354	5·315
9	—	—	5·03	5·049	5·007
10	—	—	4·72	4·755	4·714
11	—	—	4·44	4·476	4·438
12	4·270	4·28	4·15	4·213	4·180
13	—	—	—	—	3·938
14	—	—	—	—	3·713
15	—	—	—	—	3·504
16	—	—	—	—	3·309
17	—	—	—	—	3·130
18	3·041	3·013	—	2·996	2·963
19	—	2·86	—	2·86	2·809

Table 7. Intermediate energy elastic integral (a) and momentum transfer (b) cross sections (πa_0^2).

	R-matrix calculation (present)		Scott and Taylor (1979)	LaBahn and Callaway (1979)	Register *et al* (1980)		de Heer and Jansen (1977)
E(eV)	(a)	(b)	(a)	(a)	(a)	(b)	(a)
20	3·442	3·028	—	3·380	3·410	2·93	3·349
25	2·952	2·376	—	2·878	2·853	2·213	2·623
30	2·535	1·896	2·416	2·480	2·399	1·712	2·542
40	1·968	1·281	1·825	1·910	1·796	1·111	1·909
50	1·573	0·913	1·441	1·531	1·432	0·798	1·574
80	1·279	0·692	—	1·264	1·160	0·573	1·457
80	0·916	0·435	0·847	0·920	0·807	0·351	0·904
90	0·787	0·358	—	0·802	0·705	0·289	—
100	0·693	0·302	0·657	—	0·637	0·240	0·694
150	0·421	0·148	0·408	—	0·398	0·118	0·436
	0·305	0·083	0·292	—	0·284	0·0716	0·311

the measurements of Milloy and Crompton (1977) on the momentum transfer cross section (table 6).

At impact energies of 20 eV or more, integral elastic and momentum transfer cross sections are displayed together in table 7. Good agreement is obtained between the present calculation and experimental measurements of Register *et al* (1980) and the semi-empirical experiments of de Heer and Jansen (1977).

4. Conclusion

We have presented a calculation in which the ground-state He wavefunction is coupled only with a ^{1}P pseudo-state to allow for the full dipole polarisability. Similar calculations on the elastic scattering of electrons from hydrogen were carried out by Fon *et al* (1978) with excellent agreement with the experimental measurements. The present R-matrix calculations again achieve excellent all-round agreement with recent experimental measurements on phaseshifts, integral elastic, differential and momentum transfer cross sections over the entire energy range from 5 to 200 eV. We have established in this paper that (i) the range of application for the R-matrix calculation is extended by the averaging procedure developed by Burke *et al* (1981) and (ii) the present calculation can produce highly accurate data over the low and intermediate impact energy ranges and thus provide a standard with which the experimental measurements can be calibrated. Finally our calculation in its present simple form has been applied to study the elastic scattering of electrons from ground-state neon with success and the results will be reported in our next paper; further work is in progress on argon and krypton.

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References

Andrick D and Bitsch A 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 393–409
Berrington K A, Burke P G, Le Dourneuf M, Robb W D, Taylor K T and Vo Ky Lan 1978 *Comput. Phys. Commun.* **14** 367–412
Blum K and Burke P G 1975 *J. Phys. B: Atom. Molec. Phys.* **8** L410–3
Bransden B H and Hutt P K 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 603–11
Bransden B H and McDowell M R C 1969 *J. Phys. B: Atom. Molec. Phys.* **2** 1187–201
—— 1978 *Phys. Rep.* **46** 249–394
Bromberg J P 1974 *J. Chem. Phys.* **61** 963–9
Bühring W 1968 *Z. Phys.* **208** 286–98

Bullard E C and Massey H S W 1931 *Proc. R. Soc.* A **133** 637–51
Burke P G, Berrington K A and Sukumar C V 1981 *J. Phys. B: Atom. Molec. Phys.* **14** 289–305
Burke P G, Cooper J W and Ormonde S 1969 *Phys. Rev.* **183** 245–64
Burke P G and Robb W D 1972 *J. Phys. B: Atom. Molec. Phys.* **5** 44–54
Burke P G and Williams J F 1977 *Phys. Rep.* **34** 325–69
Byron F W, de Heer F J and Joachain C J 1975 *Phys. Rev. Lett.* **35** 1147–50
Byron F W and Joachain C J 1977a *Phys. Rev.* A **15** 128–46
—— 1977b *J. Phys. B: Atom. Molec. Phys.* **10** 207–26
Callaway J, LaBahn R W, Poe R T and Duxler W M, 1968 *Phys. Rev.* **168** 12–21
Crooks G B and Rudd M E 1972 *Bull. Am. Phys. Soc.* **17** 131
Duxler W M, Poe, R T and LaBahn B A 1971 *Phys. Rev.* A **4** 1935–44
Fink M and Yates A C 1970 *Atom. Data* **1** 385–456
Fon W C, Berrington K A, Burke P G and Kingston A E 1979 *J. Phys. B: Atom. Molec. Phys.* **12** 1861–72
Fon W C, Burke P G and Kingston A E 1978 *J. Phys. B: Atom. Molec. Phys.* **11** 521–30
Gerjuoy E and Krall N A 1960 *Phys. Rev.* **119** 705–11
—— 1962 *Phys. Rev.* **127** 2105–13
Gibson J R and Dolder K T 1969a *J. Phys. B: Atom. Molec. Phys.* **2** 741–6
—— 1969b *J. Phys. B: Atom. Molec. Phys.* **2** 1180–6
Gupta S C and Rees J A 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 1267–74
de Heer F J and Jansen R H J 1977 *J. Phys. B: Atom. Molec. Phys.* **10** 3741–58
Hutt P K, Islam M M, Rabheru A and McDowell M R C 1976 *J. Phys. B: Atom. Molec. Phys.* **9** 2447–60
Jansen R H, de Heer F J, Luyken H J, van Wingerden B and Blaauw H J 1976 *J. Phys. B: Atom. Molec. Phys.* **9** 185–212
Jost K, Fink M and Herrmann D 1973 *Proc. 8th Int. Conf. on Physics of Electronic and Atomic Collisions* (Beograd: Institute of Physics) Abstracts pp 269–70
Kennerly R E and Bonham R A 1978 *Phys. Rev.* A **17** 1844–54
Knowles M and McDowell M R C 1973 *J. Phys. B: Atom. Molec. Phys.* **6** 300–13
Kurepa M V and Vušković L 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 2067–78
LaBahn R W and Callaway J 1970 *Phys. Rev.* A **2** 366–9
McConkey J W and Preston J A 1975 *J. Phys. B: Atom. Molec. Phys.* **8** 63–74
Mehr J 1967 *Z. Phys.* **198** 345–50
Milloy H B and Crompton R W 1977 *Phys. Rev.* A **15** 1847–50
Moiseiwitsch B L 1977 *Rep. Prog. Phys.* **40** 843–904
Moiseiwitsch B L and Smith F J 1968 *Rev. Mod. Phys.* **40** 238–321
Nacache P F and McDowell M R C 1974 *J. Phys. B: Atom. Molec. Phys.* **7** 2382–95
Nesbet R K 1979 *Phys. Rev.* A **20** 58–70
O'Malley T F, Burke P G and Berrington K A 1979 *J. Phys. B: Atom. Molec. Phys.* **12** 953–65
Ramsauer C and Kollath R 1932 *Ann. Phys., Lpz* **12** 529–61
Register D F, Trajmar S and Srivastava S K 1980 *Phys. Rev.* A to be published
Rosenberg L, O'Malley T F and Spruch L 1961 *J. Math. Phys.* **2** 491–8
Scott T and Taylor H S 1979 *J. Phys. B: Atom. Molec. Phys.* **12** 3385–97
Sethuraman S K, Rees J A and Gibson J R 1974 *J. Phys. B: Atom. Molec. Phys.* **7** 1741–7
Sinfailam A L and Nesbet R K 1972 *Phys. Rev.* A **6** 2118–25
Srivastava S K and Trajmar S 1976 *J. Chem. Phys.* **64** 3886–8
Stein T S, Kauppila W E, Pol V, Smart J H and Jesion G 1978 *Phys. Rev.* A **17** 146–54
Steph N C, McDonald L and Golden D E 1979 *J. Phys. B: Atom. Molec. Phys.* **12** 1507–27
Walker D W 1971 *Adv. Phys.* **20** 257–323
Wichmann E and Heiss P 1974 *J. Phys. B: Atom. Molec. Phys.* **7** 1042–51
Williams J F 1979 *J. Phys. B: Atom. Molec Phys.* **12** 265–82
Winters K H, Clark C D, Bransden B H and Coleman J P 1974 *J. Phys. B: Atom. Molec. Phys.* **7** 788–98
Yarlagadda B S, Csanak G, Taylor H S, Schneider B and Yaris R 1973 *Phys. Rev.* A **7** 146–54
Yau A W, McEachran R P and Stauffer A D 1978 *J. Phys. B: Atom. Molec. Phys.* **11** 2907–22