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The elastic scattering of electrons from inert gases: III. Argon†

W C Fon‖§, K A Berrington‡, P G Burke‖‡ and A Hibbert‡

‖ Science and Engineering Research Council, Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, England

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

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Abstract. The calculations of Fon *et al* on electron–helium and electron–neon elastic scattering in which the atomic ground-state wavefunction is coupled with a ^{1}P pseudo-state to include the full dipole polarisability, are extended to consider the elastic scattering of electrons from argon. Phaseshifts, differential, integral and momentum transfer cross sections for electrons elastically scattered from argon are reported for impact energies ranging from 3 to 150 eV. A critical assessment of previous theories and experimental measurements is made.

1. Introduction

This paper is the third in a series which studies phaseshifts, integral, differential and momentum transfer cross sections of electrons elastically scattered from inert-gas atoms calculated using the R-matrix method described in paper I (Fon *et al* 1981) and paper II (Fon and Berrington 1981).

The scattering of electrons from inert gases has attracted considerable theoretical and experimental interest in recent years. This is partly due to recent developments in rare-gas–halide high-power lasers and partly due to the fact that accurate experiments are possible for these gases providing a stringent test of the theoretical models. The pronounced double-dip feature which shows up in the elastic differential cross sections in argon and krypton has always provided a strong challenge to experimentalists and theoreticians alike to obtain the positions and magnitudes of the cross sections correctly at these dips.

Although many measurements of relative differential cross sections for the elastic scattering of electrons by Ar have been reported since the early 1930s (Arnot 1931, Webb 1935), the angular resolution obtained was poor and the results were not of the highest accuracy (see Bransden and McDowell 1978, Kieffer 1971). These were followed by the works of Mehr (1967), Schackert (1968), Dudler (1973) and Lewis *et al* (1974). Unfortunately these earlier measurements were not absolute and only recently Andrick (1973), Williams and Willis (1975), Gupta and Rees (1975), Vuskovic and Kurepa (1976), DuBois and Rudd (1976) and Jansen *et al* (1976) have reported absolute elastic differential cross sections for Ar at intermediate energies.

† This paper is dedicated to Professor M J Seaton on the occasion of his 60th birthday.

§ SERC Senior Research Associate on research leave from the Department of Mathematics, University of Malaya, Kuala Lumpur, Malaysia.

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Among these absolute measurements, those of Williams and Willis are, perhaps, the most extensive and are in excellent agreement in shape with the relative data of Lewis *et al* (1974). However they are appreciably smaller than those of Jansen *et al* (1976) above 100 eV at scattering angles $\theta < 50°$, which in turn are in excellent agreement with the measurements of Bromberg (1974) at high energies. The most recent measurements of Srivastava *et al* (1981) again are substantially higher than those of Williams and Willis (1975). Therefore it is of interest to perform an independent *ab initio* calculation to compare with these absolute measurements. Unfortunately, there are few accurate calculations. Although simple model potential scattering calculations of Furness and McCarthy (1973), McCarthy *et al* (1977) and Berg *et al* (1971) do provide reasonable fits to the experimental data, they should not be viewed in the same light as calculations in which the polarisation and correlation effects are included in an *ab initio* way. Walker (1971) has also obtained improved agreement with experiment at low and intermediate energies using relativistic calculations. However, at high energies ($E \leqslant 400$ eV) these calculations, although giving an accurate account of the angular dependence of observations, are about a factor of two larger. There is, moreover, little evidence to suggest that relativistic effects are contributing significantly to the elastic scattering of electrons from argon at these energies.

Another approach has been based on the polarised-orbital approximation. Elastic calculations for argon have been carried out by Thompson (1971), Garbaty and LaBahn (1971) and Yau *et al* (1978, 1980). This method includes non-adiabatic effects only approximately and makes no allowance for inelastic effects which occur at higher energies and which become increasingly important for heavier atoms. Thus it is found that while the polarised-orbital method is quite successful for low-energy scattering from helium and neon, it becomes less successful for heavier atoms like argon and krypton particularly at the intermediate energies considered in this paper.

Pindzola and Kelly (1974) and Amusia *et al* (1982) have also calculated the cross sections and phaseshifts for the elastic scattering of electrons on neutral argon using many-body perturbation theory and the simplified random-phase approximation with exchange to obtain the optical potential. In principle these approaches give a complex non-local potential since exchange, non-adiabatic and absorption effects are included. However so far only a limited number of results have been reported and a detailed comparison with recent experiments at intermediate energies has not been made.

In this paper, we shall assume that the spin–orbit interaction and other relativistic effects are not significant in the elastic scattering of electrons on neutral argon. The polarisation, exchange and absorption effects are built in a natural way by coupling the argon ground state to a ^{1}P pseudo-state. The present paper thus represents an *ab initio* attempt to obtain elastic scattering cross sections of electrons on argon atoms over a wide range of energies (3 to 150 eV), which, while not expected to be of the highest accuracy, should give a reasonable representation of the essential physical features of the cross sections.

2. *R*-matrix calculation

In this paper the R-matrix program described by Berrington *et al* (1978) is used to calculate the phaseshifts and K-matrix elements. The R-matrix radius is taken to be 9 au and the number of continuum orbitals included for each angular momentum is 13. The calculations were carried out by coupling the Ar ground-state wavefunction

with a ^{1}P pseudo-state to allow for the ground-state static dipole polarisability. This requires the solution of a problem with two coupled channels when the total angular momentum $L = 0$ and three coupled channels when $L \geqslant 1$. While the Hartree–Fock (HF) Ar ground-state wavefunction is given in Clementi and Roetti (1974), the ^{1}P pseudo-state is expressed as linear combination of four configurations, namely

$$a_1(1s^2 2s^2 2p^6 3s 3p^6 4\bar{p}) + a_2(1s^2 2s^2 2p^6 3s^2 3p^5 4\bar{s}) + a_3(1s^2 2s^2 2p^6 3s^2 3p^5 4\bar{d}) + a_4(1s^2 2s^2 2p^6 3s^2 3p^5 3\bar{d}) \quad (1)$$

where $a_1 = 0.086\,00$, $a_2 = -0.522\,23$, $a_3 = -0.555\,64$, $a_4 = 0.641\,20$.

The one-electron radial orbitals are expressed in the form

$$P_{nl}(r) = \sum_i C_i r^{P_i} \exp(-\xi_i r). \quad (2)$$

The parameters $\{C_i\}\{P_i\}$ and $\{\xi_i\}$ for 1s, 2s, 2p, 3s and 3p were taken from Clementi and Roetti (1974). The parameters for the other orbitals are given in table 1. Those

Table 1. Values of parameters for the pseudo-orbitals.

Orbital	C_i	P_i	ξ_i
$3\bar{d}$	6.871 71	3	2.219 84
$4\bar{s}$	6.489 11	1	14.095 72
	−24.650 59	2	6.109 93
	10.597 10	3	2.988 23
	−0.345 13	4	1.269 30
$4\bar{p}$	53.834 77	2	7.503 55
	−12.579 33	3	2.032 39
	6.794 51	4	1.992 54
$4\bar{d}$	4.022 33	3	2.064 17
	−0.588 64	4	1.362 59

for the $3\bar{d}$ are determined by optimising the ground-state energy including near-degeneracy effects, using the CIV3 program of Hibbert (1975). Those for the pseudo-orbitals $4\bar{s}$, $4\bar{p}$, $4\bar{d}$ were determined by optimising the ground-state static dipole polarisability following Vo Ky Lan *et al* (1976) using the code CIVPOL with a single configuration ground state and a ^{1}P pseudo-state defined by (1). The ground-state energy is −526.817 391 au while the CI wavefunction for the ^{1}P pseudo-state gives a polarisability equal to 12.7875 au. This compares with the experimental value of 11.0 au (Landolt-Börnstein 1950). At very low energies, the scattering is sensitive to the polarisability of the atom. The present calculation may thus be unreliable at energies below about 5 eV, since our static dipole polarisability is not highly accurate and contributions from higher multipoles which may also play a role are not included.

In the present calculation, only partial waves up to $L = 12$ are calculated directly by the R-matrix program; for $L \geqslant 13$, the T-matrix elements converge well (see table 3) to those obtained using the effective range theory (ERT) of Rosenberg *et al* (1961)

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

where α is the calculated static dipole polarisability. Hence we can obtain T-matrix elements using

$$T_L = 2i \tan \delta_L - 2(\tan \delta_L)^2. \tag{4}$$

For energies of 100 eV and above, a few more partial waves ($L \geqslant 13$) are extrapolated to give smooth convergence to the ERT values. The highest partial wave included is $L = 400$ for $E = 150$ eV.

Pseudo-resonances due to the ^{1}P pseudo-threshold at 19.55 eV and to the $(N+1)$ electron correlation terms occur over the energies ranging from 19 to 50 eV. The T-matrix elements for impact energies in this region are extracted by an averaging technique described in a previous paper (Burke *et al* 1981). Finally we note that above the ^{1}P pseudo-threshold the pseudo-state can be excited. This makes some allowance for inelasticity effects in our calculation.

3. Results and discussion

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

$$e + Ar(^1S_0) \rightarrow e + Ar(^1S_0)$$

at impact energies ranging from 3 to 150 eV. The present calculations are given in tables 2 to 6, and figures 1 to 8, where comparisons between the present calculation and other theoretical calculations and experimental measurements are also made.

Table 2. Phaseshifts in radians for the elastic scattering of electrons from argon atoms.

E (eV)	k^2 (Ryd)	δ_0	δ_1	δ_2	δ_3	δ_4
3.00	0.220 51	−0.4866	−0.1480	0.1131	0.0264	0.0124
3.40	0.249 91	−0.5410	−0.1797	0.1353	0.0297	0.0140
4.00	0.294 0	−0.6171	−0.2258	0.1724	0.0346	0.0164
4.90	0.360 0	−0.7209	−0.2912	0.2362	0.0419	0.0199
5.00	0.367 50	−0.7320	−0.2984	0.2440	0.0427	0.0203
6.02	0.442 48	−0.8355	−0.3668	0.3294	0.0509	0.0243
6.67	0.490 30	−0.8956	−0.4075	0.3899	0.0563	0.0269
7.00	0.514 52	−0.9245	−0.4274	0.4222	0.0590	0.0282
7.50	0.551 30	−0.9668	−0.4565	0.4732	0.0632	0.0302
8.00	0.588 0	−1.0072	−0.4845	0.5261	0.0674	0.0322
8.70	0.639 47	−1.0614	−0.5219	0.6029	0.0734	0.0350
9.00	0.661 52	−1.0838	−0.5373	0.6358	0.0760	0.0363
10.00	0.735 0	−1.1554	−0.5865	0.7568	0.0849	0.0404
11.00	0.808 5	−1.2228	−0.6323	0.8730	0.0941	0.0445
12.00	0.882 0	−1.2861	−0.6753	0.9914	0.1036	0.0488
13.00	0.955 53	−1.3454	−0.7156	1.1057	0.1135	0.0530
14.00	1.029 0	−1.4006	−0.7534	1.2129	0.1239	0.0574
15.00	1.102 5	−1.4519	−0.7889	1.3114	0.1347	0.0619
16.00	1.176 0	−1.4997	−0.8219	1.4002	0.1462	0.0666
17.00	1.249 54	−1.5445	−0.8523	1.4795	0.1585	0.0713
18.00	1.322 82	−1.5870	−0.8792	1.5500	0.1724	0.0762

3.1. Phaseshifts

In table 2, the present calculated phaseshifts for $L = 0, 1, 2, 3, 4$ are presented and these are compared in figure 1 with the polarised-orbital calculations of Yau *et al* (1978, 1980) and those obtained through phaseshift analysis from experimental measurements of Williams (1979), Andrick (1973) and Srivastava *et al* (1981).

In figure 1(*a*) the present *R*-matrix calculations of s and p wave phaseshifts are seen to be in good agreement with those of Andrick (1973) but are below those of Williams (1979) while the calculations of Yau *et al* (1978) agree with those of Williams

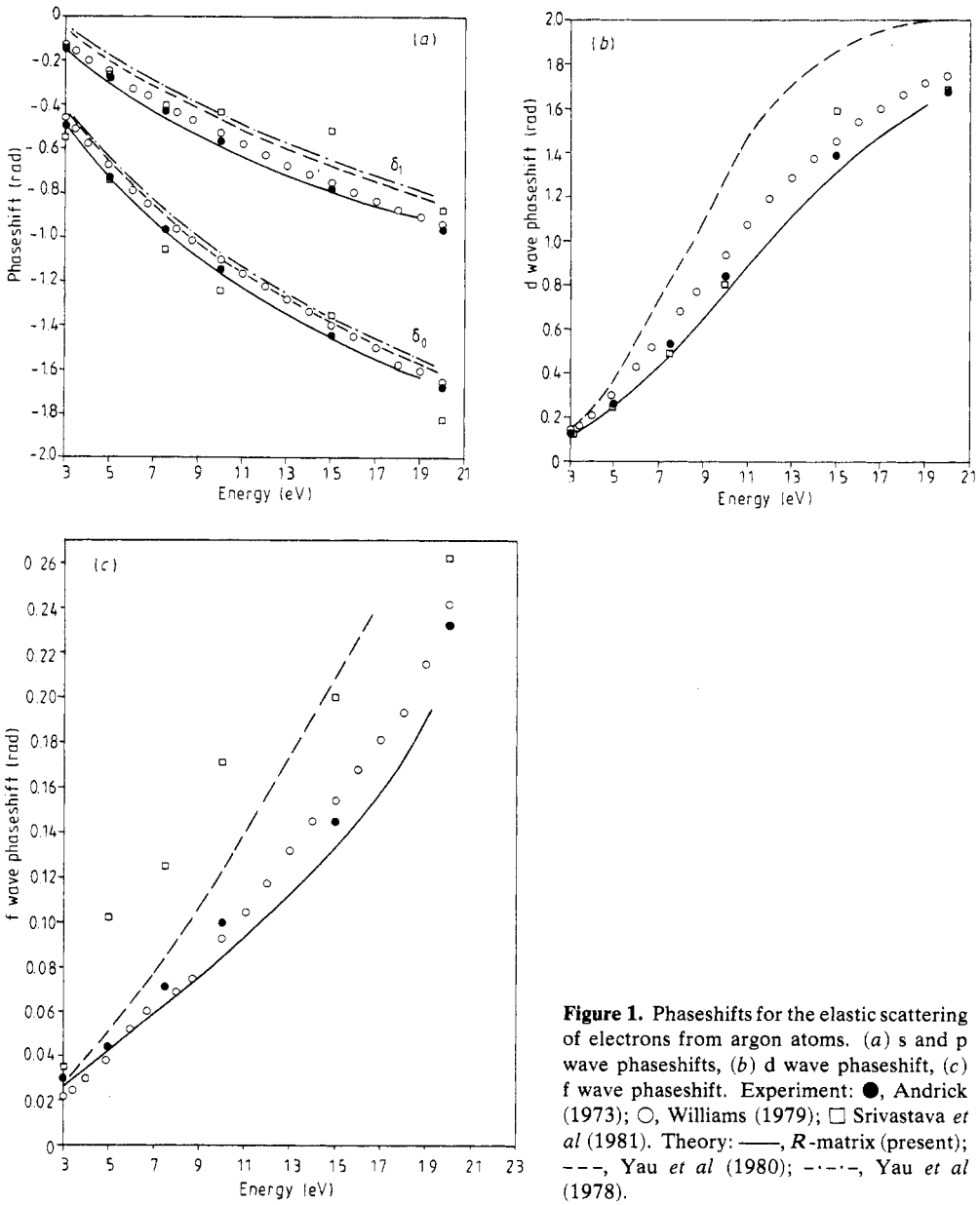

Figure 1. Phaseshifts for the elastic scattering of electrons from argon atoms. (*a*) s and p wave phaseshifts, (*b*) d wave phaseshift, (*c*) f wave phaseshift. Experiment: ●, Andrick (1973); ○, Williams (1979); □ Srivastava *et al* (1981). Theory: ——, *R*-matrix (present); – – –, Yau *et al* (1980); –·–·–, Yau *et al* (1978).

for the s wave phaseshifts. Surprisingly the simplified version (frozen core) elastic scattering phaseshifts of Yau *et al* (1980) show better agreement with those of Williams than Yau *et al* (1978). The phaseshifts obtained by Srivastava *et al* exhibit irregular features which might indicate errors in their phaseshift analysis.

Figures 1(*b*) and (*c*) show the present R-matrix calculations for d and f wave phaseshifts. They are in reasonable agreement with the experimental values although tending to lie somewhat lower. On the other hand the polarised-orbital phaseshifts of Yau *et al* (1980) tend to overestimate the measurements. As the incident energy increases, the d wave becomes increasingly dominant as it goes through a resonance. We shall see later that this contributes significantly to the discrepancy between the polarised-orbital integral and differential cross section and those of experiments.

Table 3. Comparison of phaseshifts with ERT.

	$E = 3$ eV		$E = 5$ eV		$E = 10$ eV		$E = 16$ eV	
δ_L (rad)	A	B	A	B	A	B	A	B
δ_3	0.028 1	0.026 4	0.046 9	0.042 7	0.094 0	0.084 9	0.151 1	0.146 2
δ_4	0.012 8	0.012 4	0.021 3	0.020 3	0.042 6	0.040 4	0.068 3	0.066 6
δ_5	0.006 88	0.006 72	0.011 5	0.011 1	0.022 9	0.021 8	0.036 7	0.035 4
δ_6	0.004 13	0.004 07	0.006 88	0.006 73	0.013 77	0.013 26	0.022 0	0.021 3
δ_7	0.002 67	0.002 64	0.004 45	0.004 38	0.008 91	0.008 67	0.014 52	0.013 85
δ_8	0.001 83	0.001 81	0.003 05	0.003 01	0.006 09	0.005 98	0.009 75	0.009 54

A. ERT phaseshifts (with the calculated polarisability $\alpha = 12.7875$ au); B, R-matrix calculation (present).

In table 3, we compare the present R-matrix calculation for the higher partial-wave phaseshifts with those obtained using the ERT formula of Rosenberg *et al* (see equation (3)). The indication is that the present R-matrix phaseshifts converge rapidly towards the ERT values.

3.2. Integral elastic and momentum transfer cross sections

The present calculations of the integral elastic and momentum transfer cross sections are summarised in tables 4–6 and compared with other theoretical calculations and experimental measurements in table 5 and in figures 2–4.

Figure 2 shows that there is an excellent agreement between the present calculations for the integral elastic cross section and those measured by Kauppila *et al* (1976). The experimental values of Andrick (1973) are also in good accord with the present calculations. Table 5 shows that excellent agreement has been obtained between the measurements of Vuskovic and Kurepa (1976) and the present calculated values. Among the theoretical calculations, those of Pindzola and Kelly (1974) using the static potential and the relativistic calculation of Walker (1971) which includes static and exchange potentials seem to give closest agreement with the present calculations. Figure 3 indicates that the agreement between the present calculation on momentum transfer cross sections and the measurements of Andrick (1973) and Srivastava *et al* (1981) is satisfactory. As the experiments themselves have yet to show a pattern of consistency, it is too early to draw any definite conclusion at this stage. Further measurements on momentum transfer cross sections are needed.

From figure 2, it is obvious that the polarised-orbital method of Yau *et al* (1980) substantially overestimates the experimental values over the energy range from 4–17 eV. This is mainly due to the large value of their d wave phaseshifts.

Our integral elastic cross sections presented in table 5 are in good agreement with the experimental results of Vuskovic and Kurepa (1976) and are in reasonable accord with the semi-empirical results of de Heer *et al* (1979), within their quoted errors.

Table 4. Integral elastic and momentum transfer cross sections (present results) at low energies.

E (eV)	Q_E (10^{-20} m^2)	Q_T (10^{-20} m^2)
3	5.6574	4.2592
4	7.7135	6.0344
5	9.7338	7.9639
6	11.775	9.9530
7	13.871	11.889
8	16.000	13.638
9	18.034	15.022
10	20.051	16.092
11	21.585	16.515
12	22.764	16.482
13	23.452	16.004
14	23.661	15.201
15	23.466	14.214
16	22.968	13.164
17	22.269	12.139
18	21.466	11.205

Table 5. Integral elastic cross section (in units of a_0^2) for electron–argon scattering at intermediate energies.

E (eV)	A	B	C	D	E	F	G	H	I	J
20	68.18	74.15		71.31	68.4	71.3	68.5	69.02	69.72	68.7
30	48.95	49.10		47.21		52.2	49.0	50.10	51.22	42.4
40	38.24	33.96		32.38		41.6	37.7	38.08	41.66	31.6
50	30.77	27.65		26.48	25.6	35.1	31.1	30.90	35.66	26.7
60	26.35	24.28	26.98			30.8	26.4	26.31	31.41	22.6
70	23.28	21.95	24.41			27.4	22.8	23.16		19.7
80	21.07	19.60	21.87			25.0	20.6	20.87		18.0
90	19.14	17.89	18.87			23.1	18.9	19.13		16.5
100	17.66	17.36	17.33	18.66	17.1	21.5	17.3	17.77	22.26	15.3
110	16.54									
120	15.60									
130	14.80									
140	14.13									
150	13.57	13.55	13.33	11.86	10.9	16.6	13.0	13.74	17.26	

A, R-matrix (present); B, semi-empirical (de Heer *et al* 1979); C, Vuskovic and Kurepa (1976); D, Williams and Willis (1975); E, DuBois and Rudd (1976); F, polarised-orbital (Thompson 1971); G, static potential (Pindzola and Kelly 1974); H, relativistic+static+exchange (Walker 1971); I, relativistic+static+exchange+polarisation (Walker 1971); J, optical model (Pindzola and Kelly 1974).

Table 6. Differential cross sections for elastic electron–argon scattering (in units of 10^{-19} cm^2 sr^{-1}) and momentum transfer cross sections (in units of 10^{-20} m^2). The superscript denotes the power of ten by which the number should be multiplied.

	E (eV)								
θ (deg)	3	5	10	15	20	30	40	50	60
0	3.929^2	1.571^3	1.032^4	1.635^4	1.437^4	1.545^4	1.746^4	1.899^4	1.968^4
5	2.481^2	1.197^3	9.036^3	1.496^4	1.299^4	1.290^4	1.387^4	1.431^4	1.436^4
10	1.666^2	9.118^2	7.727^3	1.343^4	1.168^4	1.073^4	1.071^4	1.035^4	9.882^3
20	1.952^2	6.781^2	5.487^3	1.030^4	9.110^3	7.384^3	6.180^3	5.015^3	4.201^3
30	3.689^2	7.408^2	3.709^3	7.093^3	6.394^3	4.544^3	3.390^3	2.315^3	1.738^3
40	5.842^2	9.503^2	2.450^3	4.212^3	3.786^3	2.677^3	1.667^3	9.842^2	6.746^2
50	7.664^2	1.180^3	1.720^3	2.072^3	1.724^3	1.143^3	6.363^2	3.258^2	2.047^2
55									
60	8.678^2	1.330^3	1.411^3	8.559^2	4.962^2	2.641^2	1.192^2	4.248^1	2.348^1
65	8.806^2	1.353^3	1.350^3	5.634^2	2.016^2	6.479^1	1.862^1	2.394^0	7.055^0
70	8.674^2	1.334^3	1.312^3	4.316^2	8.461^1	1.160^0	3.328^0	1.520^1	2.914^1
75	8.296^2	1.274^3	1.268^3	4.112^2	1.014^2	4.291^1	5.433^1	6.943^1	8.056^1
80	7.699^2	1.174^3	1.195^3	4.515^2	2.015^2	1.543^2	1.503^2	1.522^2	1.507^2
90	6.024^2	8.825^2	9.202^2	5.409^2	4.598^2	4.397^2	3.860^2	3.419^2	3.000^2
100	4.061^2	5.363^2	5.030^2	4.771^2	5.704^2	6.118^2	5.410^2	4.633^2	3.837^2
110	2.259^2	2.363^2	1.163^2	2.773^2	4.658^2	5.643^2	5.193^2	4.393^2	3.435^2
115									
120	9.876^1	7.684^1	1.523^1	1.616^2	2.936^2	3.532^2	3.398^2	2.826^2	2.027^2
125	6.245^1	6.979^1	1.442^2	2.250^2	2.595^2	2.349^2	2.247^2	1.841^2	1.237^2
130	4.565^1	1.150^2	4.155^2	4.085^2	2.990^2	1.386^2	1.185^2	9.516^1	5.988^1
135	4.764^1	2.103^2	8.304^2	7.267^2	4.312^2	8.345^1	3.981^1	3.319^1	2.598^1
140	6.635^1	3.493^2	1.376^3	1.179^3	6.629^2	8.206^1	2.514^0	1.175^1	3.340^1
145	9.856^1	5.222^2	2.026^3	1.746^3	9.873^3	1.385^2	1.339^1	3.783^1	8.749^1
150	1.402^2	7.163^2	2.742^3	2.396^3	1.384^3	2.476^2	7.149^1	1.107^2	1.851^2
160	2.327^2	1.108^3	4.173^3	3.747^3	2.259^3	5.642^2	2.879^2	3.554^2	4.617^2
170	3.071^2	1.406^3	5.257^3	4.804^3	2.974^3	8.666^2	5.160^2	6.060^2	7.325^2
180	3.355^2	1.516^3	5.661^3	5.204^3	3.250^3	9.899^2	6.109^2	7.096^2	8.489^2
σ_{MT}					10.10	5.455	4.053	3.481	3.122

	E (eV)								
θ (deg)	70	80	90	100	110	120	130	140	150
0	2.013^4	2.043^4	2.036^4	2.044^4	2.048^4	2.052^4	2.048^4	2.070^4	2.040^4
5	1.424^4	1.405^4	1.363^4	1.330^4	1.300^4	1.266^4	1.234^4	1.209^4	1.170^4
10	9.335^3	8.810^3	8.232^3	7.724^3	7.291^3	6.878^3	6.532^3	6.183^3	6.012^3
20	3.577^3	3.124^3	2.738^3	2.464^3	2.260^3	2.098^3	1.967^3	1.856^3	1.763^3
30	1.373^3	1.142^3	9.632^2	8.376^2	7.474^2	6.815^2	6.266^2	5.857^2	5.501^2
40	5.038^2	3.995^2	3.265^2	2.760^2	2.450^2	2.265^2	2.131^2	2.054^2	2.021^2
50	1.464^2	1.138^2	9.869^1	9.049^1	8.960^1	9.705^1	1.029^2	1.088^2	1.158^2
55		5.382^1	5.638^1	6.064^1	6.887^1	8.142^1	9.072^1	9.819^1	1.067^1
60	2.349^1	3.135^1	4.416^1	5.654^1	6.954^1	8.262^1	9.156^1	9.946^1	1.057^1
65	2.059^1	3.809^1	5.549^1	7.043^1	8.369^1	9.507^1	1.017^1	1.059^1	1.080^1
70	4.629^1	6.621^1	8.255^1	9.595^1	1.067^2	1.120^2	1.144^2	1.151^2	1.117^2
75	9.223^1								
80	1.504^2	1.573^2	1.560^2	1.534^2	1.502^2	1.411^2	1.320^2	1.232^2	1.146^2
90	2.635^2	2.368^2	2.078^2	1.839^2	1.632^2	1.393^2	1.208^2	1.062^2	9.093^1
100	3.095^2	2.525^2	1.997^2	1.590^2	1.283^2	9.855^1	7.832^1	6.370^1	5.130^1
110	2.549^2	1.841^2	1.267^2	8.808^1	6.044^1	3.858^1	2.569^1	1.813^1	1.268^1

Table 6. (continued)

	E (eV)								
θ (deg)	70	80	90	100	110	120	130	140	150
115		1.312^{2}	8.147^{1}	4.915^{1}	2.843^{1}	1.383^{1}	7.055^{0}	4.163^{0}	3.629^{0}
120	1.324^{2}	7.821^{1}	4.077^{1}	1.831^{1}	6.548^{0}	8.578^{-1}	2.770^{-1}	2.070^{0}	5.692^{0}
125	7.299^{1}	3.624^{1}	1.435^{1}	4.413^{0}	2.032^{0}	4.871^{0}	9.777^{0}	1.518^{1}	2.137^{1}
130	3.403^{1}	1.745^{1}	1.288^{1}	1.465^{1}	2.042^{1}	3.005^{1}	3.857^{1}	4.513^{1}	5.239^{1}
135	2.788^{1}	3.227^{1}	4.361^{1}	5.394^{1}	6.507^{1}	7.830^{1}	8.719^{1}	9.306^{1}	9.843^{1}
140	6.261^{1}	8.635^{1}	1.090^{2}	1.239^{2}	1.362^{2}	1.490^{2}	1.550^{2}	1.574^{2}	1.580^{2}
145	1.409^{2}								
150	2.589^{2}	3.041^{2}	3.346^{2}	3.435^{2}	3.427^{2}	3.426^{2}	3.336^{2}	3.191^{2}	3.044^{2}
160	5.673^{2}	6.134^{2}	6.315^{2}	6.134^{2}	5.863^{2}	5.608^{2}	5.271^{2}	4.912^{2}	4.550^{2}
170	8.461^{2}	8.809^{2}	8.789^{2}	8.345^{2}	7.812^{2}	7.311^{2}	6.757^{2}	6.215^{2}	5.686^{2}
180	9.554^{2}	9.756^{2}	9.690^{2}	9.189^{2}	8.543^{2}	7.955^{2}	7.307^{2}	6.696^{2}	6.063^{2}
σ_{MT}	2.888	2.679	2.489	2.309	2.165	2.044	1.931	1.828	1.730

It is interesting that if we add to our elastic cross section, the inelastic cross section for exciting our ^{1}P pseudo-state we obtain 38.9 a_0^2 at 50 eV, 27.4 a_0^2 at 100 eV and 22.4 a_0^2 at 150 eV compared with 39.8 a_0^2, 29.6 a_0^2 and 24.8 a_0^2 for the total cross section at these energies, given by de Heer *et al* (1979). From this we see that inclusion of the ^{1}P pseudo-state represents most of the inelasticity at these energies.

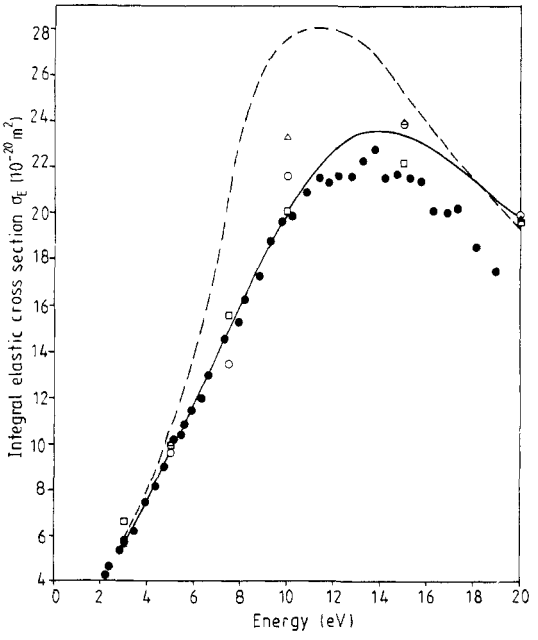

Figure 2. Integral elastic cross section (10^{-20} m^2) at low energies. Experiments: ●, Kauppila *et al* (1976); △, Williams (1979); ○, Andrick (1973); □, Srivastava *et al* (1981). Theory: ——, R-matrix (present); – – –, polarised-orbital (Yau *et al* 1980).

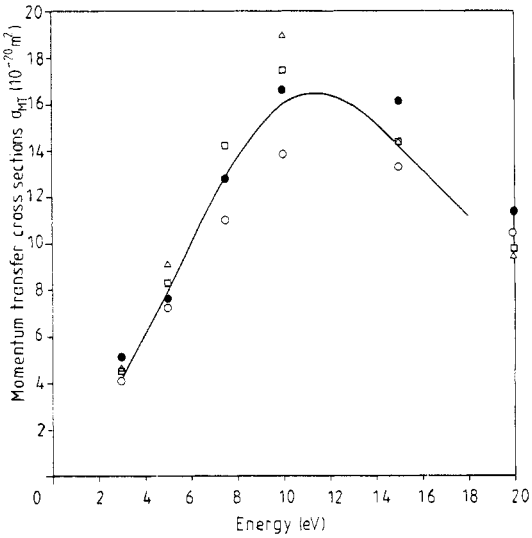

Figure 3. Momentum transfer cross section (10^{-20} m^2) at low energies. Experiment: ○, Frost and Phelps (1964); △, Williams (1979); □, Andrick (1973); ●, Srivastava *et al* (1981). Theory: ——, R-matrix (present).

3.3. Differential cross sections

The present calculation of the elastic differential cross sections is summarised in table 6. Comparison with other calculations and experiments is made in figures 4 to 8.

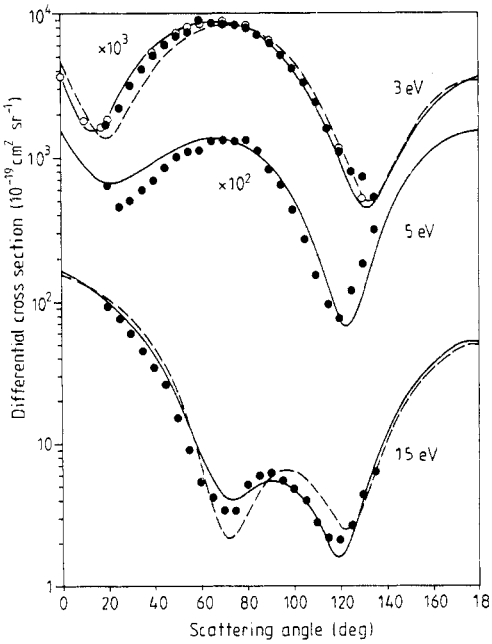

Figure 4. Differential cross section (10^{-19} cm^2 sr^{-1}) at 3, 5 and 15 eV. Experiment: ●, Srivastava *et al* (1981); ○, Andrick (1973). Theory: ——, R-matrix (present); – – –, polarised-orbital (McEachran and Stauffer 1982).

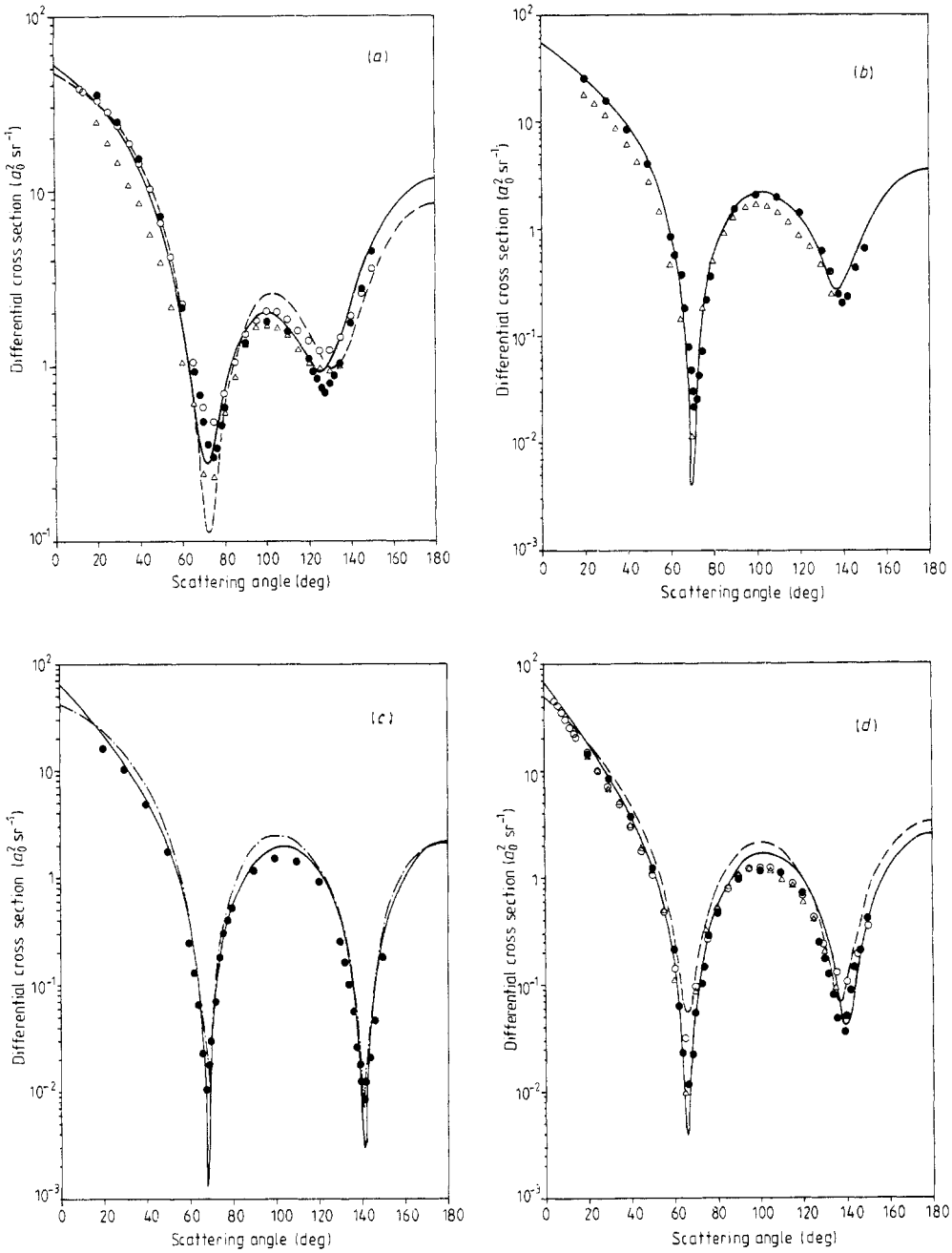

Figure 5. Differential cross section (a_0^2 sr^{-1}) at: (*a*), 20 eV; (*b*), 30 eV; (*c*), 40 eV; (*d*), 50 eV. Experiment: ●, Williams and Willis (1975); ○, DuBois and Rudd (1976); △, Srivastava *et al* (1981). Theory: ——, *R*-matrix (present); – – –, polarised-orbital (McEachran and Stauffer 1982); –·–·–, polarised-orbital (Thompson 1971).

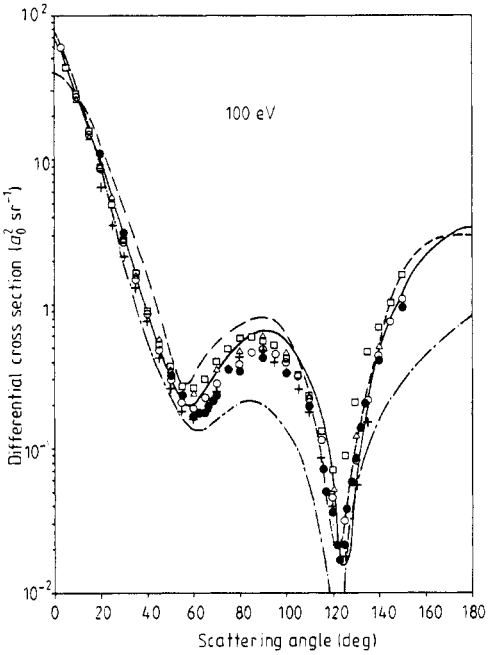

Figure 6. Differential cross section (a_0^2 sr^{-1}) at 100 eV. Experiment: ●, Williams and Willis (1975); ○, DuBois and Rudd (1976); △, Gupta and Rees (1975); +, Srivastava *et al* (1981); □, Vuskovic and Kurepa (1976). Theory: ——, R-matrix (present); – – –, Thompson (1971); –·–·–, Joachain *et al* (1977).

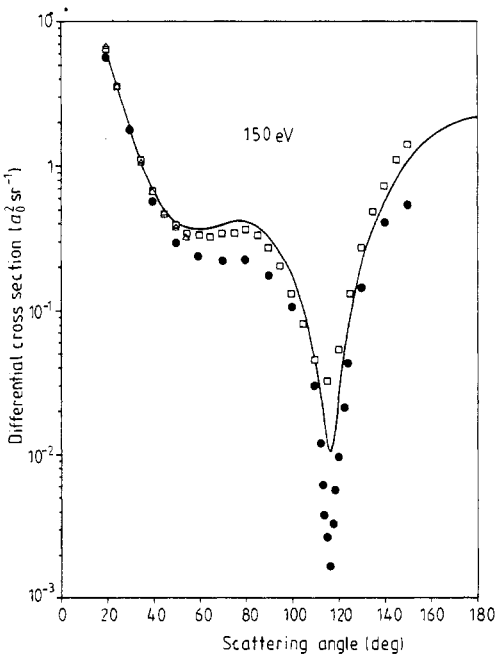

Figure 7. Differential cross section (a_0^2 sr^{-1}) at 150 eV. The legend is the same as figure 6 except that △ represents the measurements of Jansen *et al* (1976).

In accordance with the present calculation, the general features of the differential cross section show

(i) a sharp forward peak;
(ii) a peak in the backward direction;
(iii) the formation of double minima at all energies considered.

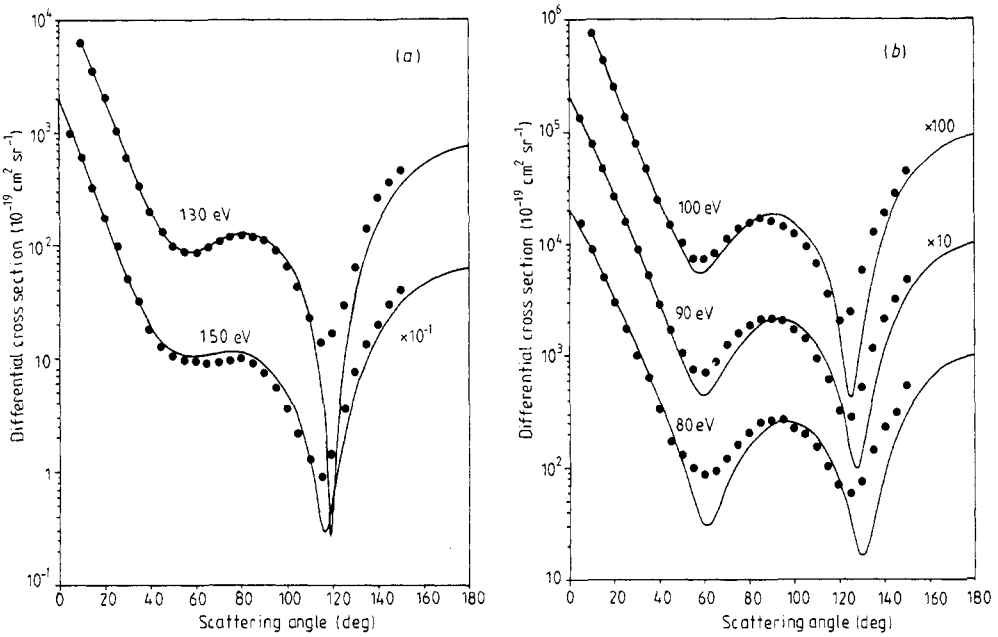

Figure 8. Differential cross section (10^{-19} cm^2 sr^{-1}) at: (*a*), 130 and 150 eV; (*b*), 80, 90 and 100 eV. Experiment: ●, Vuskovic and Kurepa (1976). Theory: ——, *R*-matrix (present).

This sharp forward peak arises mainly from high partial waves and becomes more pronounced as the incident energy increases. As the ground-state static dipole polarisability of Ar is much larger than that of He or Ne, higher partial waves are contributing to the cross section and consequently the forward peak is sharper. The double-dip formation is entirely due to the dominance of the d partial wave. At very low energies the d wave is overshadowed by the large contribution from the s and p waves. However, as energy increases, the two dips become sharper and more pronounced. At impact energy $E \geqslant 20$ eV, the first dip seems to increase its depth faster than the second, but above 40 eV, the second dip becomes deeper and the first retreats slowly. As the incident energy reaches 150 eV, the first dip fades into a shoulder and slowly disappears when the impact energy increases above 150 eV.

At 15 eV, figure 4 shows that the present *R*-matrix calculation seems to be in closer agreement with the measurements of Srivastava *et al* (1981) than the polarised-orbital calculation of McEachran and Stauffer (1982). This is basically because the present calculation predicts a smaller contribution from the d wave.

Figure 5 shows excellent agreement between the *R*-matrix calculation and the experimental measurements of Williams and Willis (1975) and DuBois and Rudd (1976). The measurements of Srivastava *et al* (1981) seem to be rather low at smaller scattering angles but otherwise there is excellent agreement in shape with the *R*-matrix calculation.

In figure 6, the *R*-matrix calculation again predicts the experimental measurements better than the polarised-orbital model of Thompson (1971) or the optical potential model of Joachain *et al* (1977). Among the experiments, the *R*-matrix calculation lies very much closer to the measurements of Vuskovic and Kurepa (1976) and those

of Gupta and Rees (1975). Discrepancy slowly creeps in between the R-matrix calculation and the measurements of Williams and Willis (1975). At 150 eV, this discrepancy becomes so pronounced that the good agreement they have at energies below 50 eV has been eroded. On the other hand, the agreement between the R-matrix calculation and the measurements of Vuskovic and Kurepa (1976) seems to improve as the impact energy increases to 130 eV (see figure 8(*a*)). What is so striking is that there is a consistent pattern of agreement between the two for all the energies measured by Vuskovic and Kurepa (1976) (see figure 8(*b*)) in particular for scattering angles less than 50°. At these scattering angles, there is no disagreement between the measurements of Vuskovic and Kurepa (1976) and those of Jansen *et al* (1976) whereas the measurements of Williams and Willis (1975) tend to drift further and further below those measured by Jansen *et al* (1976) and those of Bromberg (1974) as the incident energy increases.

Further experimental investigations are required to remove the discrepancy which exists among various experiment measurements in particular at small scattering angles as it reflects directly on the validity of the normalisation procedure.

4. Conclusion

We have demonstrated that R-matrix calculations described in papers I and II in which the ground-state wavefunction is coupled with a ^{1}P pseudo-state to include the full ground-state static dipole polarisability again produce satisfactory agreement with experiments on phaseshifts, differential, integral and momentum transfer cross sections for the elastic scattering of electrons from argon. The lack of uniform agreement among the experimental measurements over the entire intermediate energy range has been highlighted by the present investigation and we hope that this will encourage further experimental investigations. Further work on krypton is in progress.

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