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Differential and total electron scattering from neon at low incident energies

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Abstract. Absolute differential (in angle) and total scattering cross sections for low-energy (0.1–7.0 eV) electron scattering from neon have been measured. Both data sets have been analysed using phaseshift techniques and comparisons are made between the present cross sections and phaseshifts and similar data from previous swarm and beam experiments, and theory. We also discuss the present data in the context of the recent proposal by Shi and Burrow regarding the use of neon as a secondary elastic cross section 'standard'.

1. Introduction

Low-energy electron scattering from atoms and molecules is a field of substantial interest to the atomic collisions community, both from the point of view of providing accurate data to test theoretical calculations and also as a source of data for modelling an increasing number of processes which are based on low-temperature discharges or plasmas. For these purposes, particularly the former but increasingly the latter, the level of accuracy of the measured scattered cross sections is of prime importance. Most measurements of absolute elastic or inelastic (vibrational, electronic excitation) differential scattering cross sections for gaseous targets are not truly 'absolute', but rather are placed on an absolute scale by the use of some 'standard' cross section, in conjunction with the relative flow technique (Srivastava *et al* 1975). For low-energy electron scattering the 'standard' cross section which is normally used is that for electron–helium elastic scattering. This cross section has been measured extensively, the absolute values being obtained from the application of phaseshift analysis techniques, and calculated in an *ab initio* fashion by several groups, and is widely regarded as being known to within a few per cent for energies below the first inelastic threshold at 19.8 eV. To our knowledge, the same level of agreement between experiment and theory has not been demonstrated for any other atomic or molecular system.

In the light of several low-energy experimental and theoretical studies on neon (Williams 1979, O'Malley and Crompton 1980, Brewer *et al* 1981, Register and Trajmar 1984, Saha 1989, 1990, Shi and Burrow 1992) which are generally in excellent agreement with one another, Shi and Burrow have proposed that neon may be used as a 'secondary

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standard' for low-energy electron scattering. As such it is not intended that it would usurp the role of helium but rather serve as a means for checking the operation of any scattering apparatus which uses the helium cross section as a reference standard. Furthermore, recent work in this laboratory on the size and shape of pseudo-effusive beams (Buckman *et al* 1993) indicates that, at elevated driving pressures, the width of a helium beam is smaller than that of most other gases, even when the driving pressures are adjusted such that the mean free paths of the gases are identical. As the relative flow technique is based on experimental measurements carried out under identical scattering conditions for the target and reference gases, the smaller widths observed for helium beams is a matter of some concern, and serves to strengthen the case for establishing a secondary standard for low-energy scattering. The fact that Buckman *et al* did not observe any significant differences in the size of neon beams, as a function of pressure, compared with a range of other atomic and molecular gases (with the exception of helium) adds further weight to the case for its use as a secondary standard.

When one closely compares the available experimental data and theory for electron scattering from neon at energies below about 7 eV a somewhat patchy picture emerges. In the case of the differential scattering measurements, at the higher end of this energy range all of the experimental and theoretical contributions noted above appear to be in excellent agreement (±5%). However, at energies below about 2.0 eV there are some differences (10–30%) between, on the one hand, the extensive set of differential cross section (DCS) measurements of Williams (1979), and on the other the DCS measurements of Shi and Burrow (1992), the swarm-derived cross sections of O'Malley and Crompton (1980) and the *ab initio* theory of Saha (1989, 1990). In the case of the total cross section, where one may expect higher accuracy, smaller, but nonetheless significant, differences exist between some experiments (for example Salop and Nakano 1970, Nickel *et al* 1985, Kumar *et al* 1987) and theory (Dasgupta and Bhatia 1984, McEachran and Stauffer 1985, Yuan 1988, Saha 1989) over the entire energy range. In particular at higher energies (above about 4 eV) the most recent experiments by Kumar *et al* and Nickel *et al* differ by as much as 10%, with the former being in relatively good agreement with the theory of Saha up to 8 eV and the latter being larger in magnitude and in better agreement with the polarized orbital theory of McEachran and Stauffer at higher energies. In addition the swarm-derived integral cross sections of O'Malley and Crompton and those from the theory of Saha are in excellent agreement at energies below 2.2 eV, whilst at higher energies (up to 7 eV) the momentum transfer cross section of Robertson (1972) is as much as 5% larger than that predicted by Saha.

Thus the present work, a series of measurements of both differential and total elastic cross sections for electron scattering from neon at energies between 0.10 and 7.0 eV, is motivated by the need to further investigate these small but significant discrepancies and evaluate the applicability of this scattering system to serve as a secondary standard. The present work also serves to complement the work of Williams (1979), Brewer *et al* (1981) and Register and Trajmar (1984), all of whom have carried out phaseshift analyses of DCS data at higher energies. The new data provide a wider opportunity for a comparison with theory, in particular the multiconfiguration Hartree–Fock calculations of Saha, which include both polarization and correlation effects, the adiabatic-exchange (AE) calculations of McEachran and Stauffer (1983, 1985), the polarized orbital calculations of Dasgupta and Bhatia (1984) and, at the total cross section level, with the static calculations of Yuan (1988).

The experimental apparatus and techniques used for the present measurements are described briefly in the next section, the scattering cross section measurements are presented in section 3, the phaseshift analysis procedure for both cross sections is outlined in section 4, and a general discussion and comparison of all of the results is given in section 5 along with some concluding remarks.

2. Experimental apparatus and techniques

Two quite separate pieces of experimental apparatus were used for the cross section measurements described here. The differential scattering cross sections were measured with a crossed-beam apparatus which has been previously described in detail (Brunger *et al* 1991, Gulley *et al* 1993) and we will not repeat that description here. The absolute cross section scale was determined using the relative flow technique in conjunction with the 'known' helium cross section (Nesbet 1979). Relative flow rates for both gases were measured for a range of driving pressures and the pressures maintained sufficiently low such that any effects on the relative sizes of the atomic beams were negligible (Buckman *et al* 1993). The incident electron energy scale was calibrated by (i) using the position of the second peak of the N_2^- shape resonance which occurs at 2.198 eV in the elastic channel (Rohr 1977) and 2.24 eV in the excitation function for the $v=0$–1 vibrational excitation channel (Ehrhardt and Willmann 1967) and (ii) by detecting the appearance of zero-energy electrons in the elastic channel as the energy was increased through zero. The energy resolution of the electron beam was typically 50 meV.

The total cross section measurements were carried out with a linear, time-of-flight (TOF) electron attenuation spectrometer. Whilst many aspects of this apparatus have also been described previously (Buckman and Lohmann 1986), there have been several recent modifications which are worth noting. Firstly, the spectrometer is now mounted in a differentially pumped manifold such that the source optics, scattering cell and detector optics are located in separate chambers. The central chamber containing the scattering cell is pumped by a $330\ \mathrm{l\ s^{-1}}$ turbomolecular pump and the source and detector chambers are pumped by $50\ \mathrm{l\ s^{-1}}$ turbomolecular pumps. Secondly the scattering cell, which is 255 mm in length, has 1 mm entrance and exit apertures, reduced from an original size of 2 mm, which in turn reduces the acceptance angle for forward scattered electrons, averaged over the entire scattering length, to 7×10^{-4} sr. The technique for the derivation of the total scattering cross section is unchanged and is based on the Beer–Lambert attenuation law. The gas number density is determined by the use of a spinning rotor viscosity gauge. The energy resolution of the apparatus varies from an estimated 1 meV at 100 meV to 150 meV at 5.0 eV. Normal precautions were taken to avoid the effects of multiple scattering.

3. Experimental results

3.1. Total scattering

Tabulated values of the measured total scattering cross section for neon (in units of $10^{-16}\ \mathrm{cm^2}$) in the energy range 0.1–5 eV are given in table 1. The estimated uncertainty in the absolute value varies between 3 and 5%. This comprises a statistical contribution (1–3%), the uncertainty in the determination of the absolute number density (2.5%) and the uncertainty in the interaction length (1%). At each energy at least 5 and as many as 15 measurements of the cross section were made under different experimental

Table 1. Absolute total cross sections for electrons scattered by neon atoms at energies between 0.1 and 5.0 eV from TOF attenuation measurements. Except where indicated the absolute error is less than 4%.

Energy (eV)	Q_T (10^{-16} cm^2)	Error (%)	Energy (eV)	Q_T (10^{-16} cm^2)	Error (%)
0.100	0.595		0.760	1.415	
0.120	0.658	4.4	0.780	1.425	
0.140	0.690		0.800	1.446	
0.160	0.734		0.820	1.457	
0.180	0.766		0.840	1.471	
0.200	0.808	4.1	0.860	1.490	
0.220	0.845		0.880	1.502	4.4
0.240	0.878	4.4	0.900	1.506	4.0
0.250	0.884	5.0	0.920	1.511	4.4
0.360	1.042		0.940	1.520	
0.380	1.057		0.960	1.544	
0.400	1.084		0.980	1.559	
0.420	1.105		1.00	1.569	
0.440	1.133		1.25	1.708	
0.460	1.153		1.50	1.827	
0.480	1.177		1.75	1.944	4.3
0.500	1.200		2.00	2.060	
0.520	1.227		2.25	2.160	
0.540	1.238		2.50	2.260	
0.560	1.262		2.75	2.339	
0.580	1.276		3.00	2.425	
0.600	1.291		3.25	2.488	
0.620	1.311		3.50	2.569	
0.640	1.326		3.75	2.617	
0.660	1.341		4.00	2.691	
0.680	1.354		4.25	2.752	
0.700	1.371		4.50	2.812	
0.720	1.360		4.75	2.852	
0.740	1.413	4.0	5.00	2.902	

conditions and the statistical figure represents the standard deviation of the set of measurements at each energy. In general this figure is somewhat larger than the raw statistical uncertainty and we believe that it gives a more realistic indication of probable systematic variations in the experiment.

The present measured total cross section is shown in figures 1(*a*) and (*b*) where it is compared with a number of recent experimental and theoretical determinations. Between 0.1 and 1.0 eV the data are tabulated in 20 meV intervals but for the sake of clarity in the figure we present them at 30 meV intervals. At energies below 2 eV (figure 1(*a*)), the present results are in excellent (±2%) agreement with the derived cross section of O'Malley and Crompton and with the theories of Saha and McEachran and Stauffer, whilst they are uniformly higher than the theory of Yuan by about 10%. The present cross section is also in excellent agreement with the measurements of Salop and Nakano, but somewhat higher (5–10%) than those of both Kumar *et al* (1987) and Sinapius *et al* (1980). For energies above 2 eV (figure 1(*b*)), the present cross section gradually departs from the theoretical cross sections—at 5 eV it is about 7% and 5% higher than Saha and McEachran and Stauffer respectively. It is systematically higher than the experimental values of Kumar *et al* but it is in good agreement with the measurement of Nickel *et al* (1985). These differences will be discussed further in section 5.

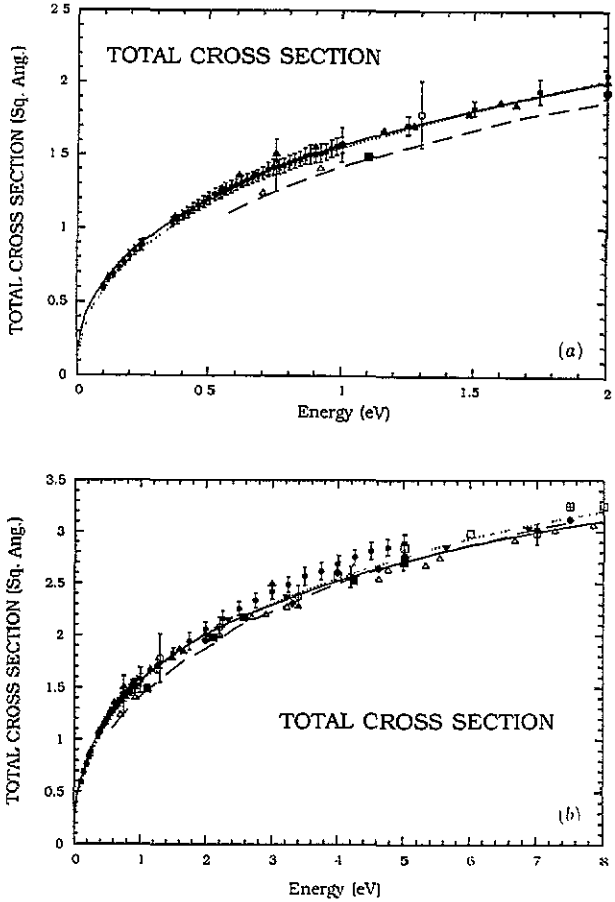

Figure 1. Total cross section in units of Å^2 for electron scattering from neon (*a*) 0–2 eV; (*b*) 0–8 eV. Present results (●) TOF measurements, (○) derived from DCS measurements; (△) Kumar *et al*; (▲) Salop and Nakano; (◆) Stein *et al*; (■) Sinapius; (▼) Charlton *et al*; (□) Nickel *et al*; (- - -) O'Malley and Crompton; (— —) Yuan; (-----) McEachran and Stauffer; (——) Saha.

3.2. *Differential scattering*

The absolute differential cross sections (in units of 10^{-16} cm^2 sr^{-1}) at energies of 0.75, 1.0, 1.3, 2.2, 3.4, 4.2, 5.0 and 7.0 eV are presented in table 2. At most energies the cross sections have been measured at 5° intervals over the range 10–130° to better facilitate the phaseshift analysis. Comparisons can be made at each energy with the theory of Saha, at energies below 2.2 eV with the derived cross sections of O'Malley and Crompton (1980), at energies above 0.58 eV with the cross sections of Williams (1979), and at selected energies with the measurements of Shi and Burrow (1992) and Register and Trajmar (1984). Whilst the energies at which the current measurements have been carried out do not always correspond to those published by others, in most cases this has been overcome by fitting the published low-order phaseshifts of these investigators to enable cross sections to be generated at any energy. This has been applied to the phaseshifts of Saha (1989), Williams (1979), O'Malley and Crompton (1980), Dasgupta and Bhatia (1984) and McEachran and Stauffer (1985). Various analytical forms have

Table 2. Absolute differential cross sections in units of $10^{-16}\,cm^2\,sr^{-1}$ for electron scattering from neon. Figures in brackets indicate the absolute uncertainty expressed as a percentage.

Angle	Energy (eV)							
(deg)	0.75	1.0	1.3	2.2	3.4	4.2	5.0	7.0
15	—	—	0.0880 (7.4)	—	0.167 (7.4)	0.190 (7.9)	0.222 (6.7)	0.254 (6.4)
20	—	—	0.0970 (8.0)	0.142 (7.6)	0.191 (6.6)	0.222 (6.7)	0.243 (10.5)	0.293 (6.4)
25	—	—	0.108 (7.8)			0.243 (6.5)	0.281 (7.4)	0.323 (6.7)
30	0.0831 (14.8)	0.0871 (12.8)	0.121 (7.7)	0.171 (7.2)	0.233 (6.7)	0.264 (6.4)	0.291 (8.6)	0.347 (6.4)
35	0.0927 (12.7)	0.107 (12.3)	0.128 (7.0)			0.283 (7.7)	0.321 (9.5)	0.379 (6.4)
40	0.0965 (15.0)	0.111 (9.9)	0.139 (6.9)	0.198 (6.5)	0.262 (6.7)	0.302 (6.4)	0.329 (6.8)	0.396 (6.6)
45	0.103 (13.0)	0.116 (9.1)	0.146 (7.3)			0.315 (6.4)	0.345 (7.1)	0.400 (6.5)
50	0.111 (11.0)	0.125 (6.9)	0.153 (6.9)	0.209 (6.7)	0.286 (6.4)	0.314 (7.7)	0.358 (6.8)	0.413 (6.8)
55	0.117 (10.0)	0.128 (6.7)	0.159 (7.0)			0.322 (6.4)	0.353 (6.9)	0.403 (6.4)
60	0.116 (11.7)	0.135 (7.7)	0.161 (7.3)	0.215 (6.4)	0.285 (6.5)	0.325 (7.2)	0.350 (7.4)	0.404 (7.0)
65	0.119 (7.2)	0.139 (7.8)	0.164 (7.4)			0.309 (6.6)	0.337 (6.7)	0.387 (7.3)
70	0.125 (9.19)	0.137 (8.2)	0.165 (6.6)	0.214 (6.4)	0.274 (6.5)	0.302 (6.8)	0.327 (9.0)	0.369 (6.5)
75	0.124 (9.6)	0.139 (9.2)	0.164 (7.4)			0.291 (6.6)	0.308 (8.0)	0.350 (6.8)
80	0.127 (12.1)	0.141 (6.5)	0.170 (7.3)	0.203 (6.5)	0.251 (6.4)	0.272 (6.5)	0.292 (7.8)	0.316 (6.9)
85	0.127 (7.34)	0.145 (8.6)	0.163 (7.5)			0.258 (7.3)	0.269 (6.7)	0.291 (7.6)
90	0.127 (12.2)	0.145 (7.9)	0.158 (7.6)	0.184 (6.5)	0.218 (6.4)	0.233 (6.6)	0.244 (6.8)	0.258 (6.9)
95	0.133 (8.7)	0.137 (8.9)	0.157 (7.2)			0.216 (6.5)	0.217 (7.0)	0.231 (6.6)
100	0.132 (8.5)	0.140 (8.7)	0.156 (8.4)	0.171 (6.5)	0.186 (6.4)	0.193 (6.5)	0.194 (8.4)	0.198 (6.7)
105	0.124 (8.05)	0.136 (7.0)	0.149 (7.8)			0.176 (6.7)	0.174 (7.2)	0.170 (7.0)
110	0.126 (8.9)	0.135 (7.4)	0.147 (7.8)	0.149 (6.4)	0.152 (6.4)	0.156 (6.6)	0.155 (6.5)	0.140 (6.8)
115	0.126 (8.3)	0.132 (8.4)	0.142 (7.5)			0.136 (6.7)	0.135 (9.9)	0.118 (6.8)
120	0.128 (7.8)	0.128 (6.7)	0.141 (8.6)	0.131 (6.5)	0.121 (6.5)	0.119 (6.5)	0.119 (8.8)	0.102 (7.7)
125	0.119 (7.6)	0.126 (7.7)	0.133 (7.7)			0.105 (6.6)	0.101 (8.3)	0.0795 (8.4)
130	0.118 (7.6)	0.129 (7.2)	0.134 (11.7)	0.116 (6.6)	0.0968 (6.4)	0.092 (7.0)	0.0832 (10.1)	0.0696 (6.9)

been investigated for this process but generally a fourth- or fifth-order polynomial fit sufficed. Higher-order phases were generated using equations (3) to (6) in the following section. The fitting process itself has no significant effect on the visual comparison offered in the figures. In the interests of brevity we do not show the results of Dasgupta and Bhatia as they are generally very similar in shape and absolute magnitude to those of McEachran and Stauffer, particularly at higher energies.

At 0.75 eV (figure 2(*a*)), the present experimental cross section is compared with that calculated from the interpolated phaseshifts of Williams (1979), O'Malley and Crompton (1980) and Saha (1989) and with the cross section of McEachran and Stauffer (1985). At this energy there are substantial differences (~15%) between the cross section of Williams (1979) and those of Saha and O'Malley and Crompton (which are essentially identical) and McEachran and Stauffer. These differences manifest themselves mainly at backward scattering angles (>~60°). For angles greater than about 60° the present cross section is in good agreement with both theories and with the swarm-derived result. At forward angles (<~50°), however, the present data tends to favour the cross section of Williams.

At 1.0 eV (figure 2(*b*)) we compare our measured cross section with that of Shi and Burrow as well as with those discussed above. The present result is once again in excellent agreement with both theories and the swarm-derived result, and this agreement extends over the entire common angular range. There is also an excellent level of agreement with the data of Shi and Burrow at all angles. Whilst there is overlap within the error bounds of the present measurements with the cross section of Williams at most angles, it is clear that there is a noticeable difference in shape between the two.

Figure 2(*c*) shows the comparison of the present DCS at 1.3 eV with that of Williams and O'Malley and Crompton and with the theories of Saha and McEachran and Stauffer. The level of agreement of the present experiment with all of the above is generally good—within the absolute experimental uncertainty—although the present cross section exhibits a slightly different shape from both those of O'Malley and Crompton and Saha, which are essentially identical, and Williams. Unfortunately, in the region in which the differences between Williams and Saha are greatest, at angles less than about 70°, the present data lie midway between the two and do not offer any resolution of this discrepancy at this energy. They do, however, continue the trend which sees the present DCS measurements lying a little higher in absolute magnitude than both the theory and swarm results at low energies and forward angles.

Figure 2(*d*) illustrates the elastic DCS at an energy of 2.2 eV where a similar series of comparisons are made. The agreement with both Saha and O'Malley and Crompton is excellent over the entire angular range. For angles greater than about 70° there is also excellent agreement with the cross section of Williams but, at smaller scattering angles, the present cross section is about 5–10% lower than that of Williams. The cross section of McEachran and Stauffer, whilst essentially identical in shape to the present, appears to be shifted to higher angles by about 5°. A similar, but less pronounced situation is seen at 3.4 eV in figure 3(*a*).

At 4.2 eV (figure 3(*b*)) there is excellent agreement with the theory of Saha (typically within ±1%) over the entire angular range. At this energy, and at the higher energies up to 7 eV, the cross sections of Saha, Williams and McEachran and Stauffer all lie within about ±5% of one another and so their level of agreement with the present experiment is also good.

At 5 eV (figure 3(*c*)), we are once again able to compare the present data with the measurements of Shi and Burrow and the lowest energy measurement in a series by

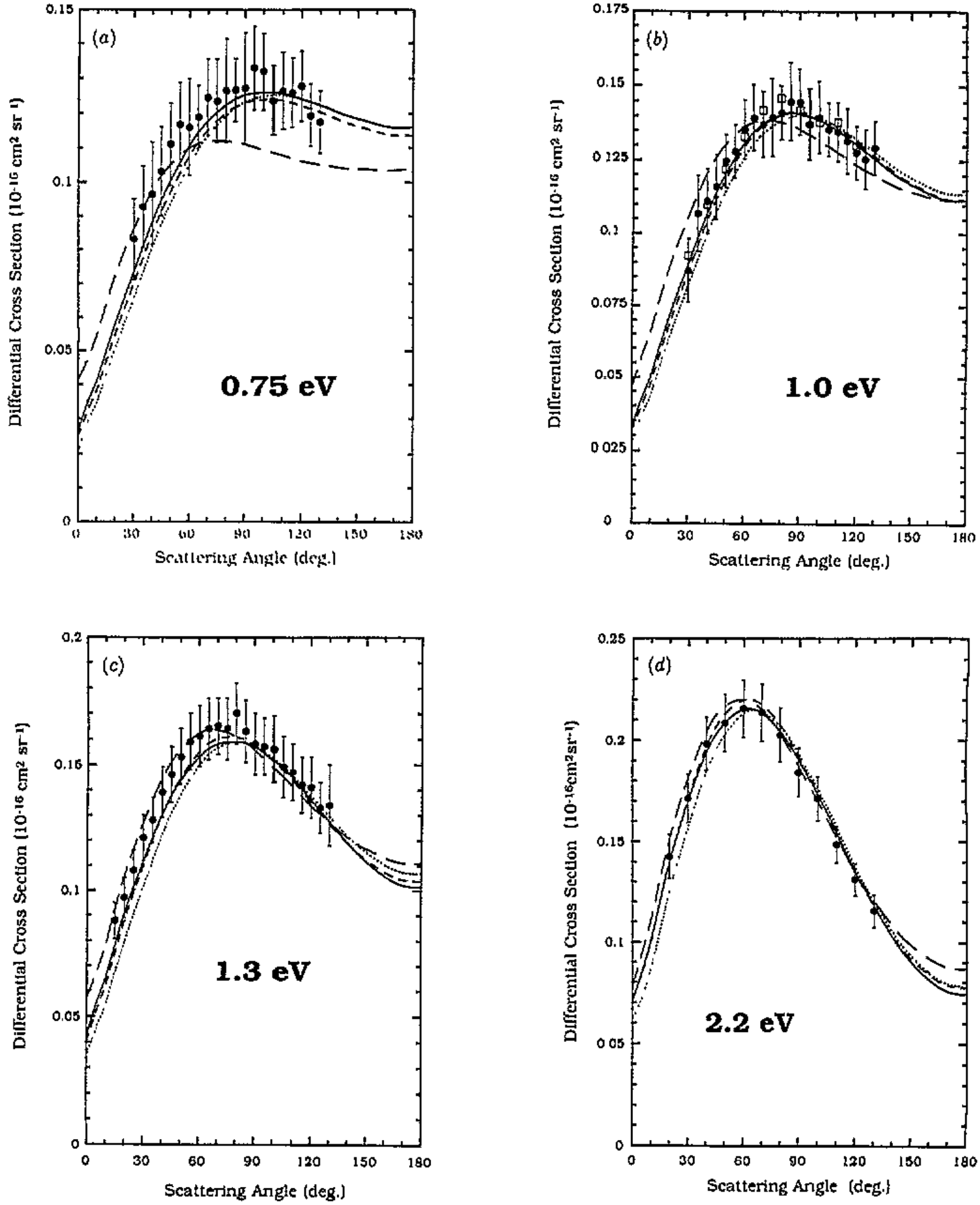

Figure 2. Differential cross sections, in units of $10^{-16}\ cm^2\ sr^{-1}$, for electron scattering from neon at (*a*) 0.75 eV, (*b*) 1.0 eV, (*c*) 1.3 eV and (*d*) 2.2 eV: (●) present results; (□) Shi and Burrow; (— —) Williams; (- - -) O'Malley and Crompton; (-----) McEachran and Stauffer; (——) Saha.

Register and Trajmar. There is excellent agreement between the present cross section and both of these measurements, although the present cross section and that of Shi and Burrow appear to be systematically higher than that of Register and Trajmar by a few per cent near the peak in the cross section between 50 and 70°. The present data are also in excellent agreement with the theory of Saha over the entire angular range,

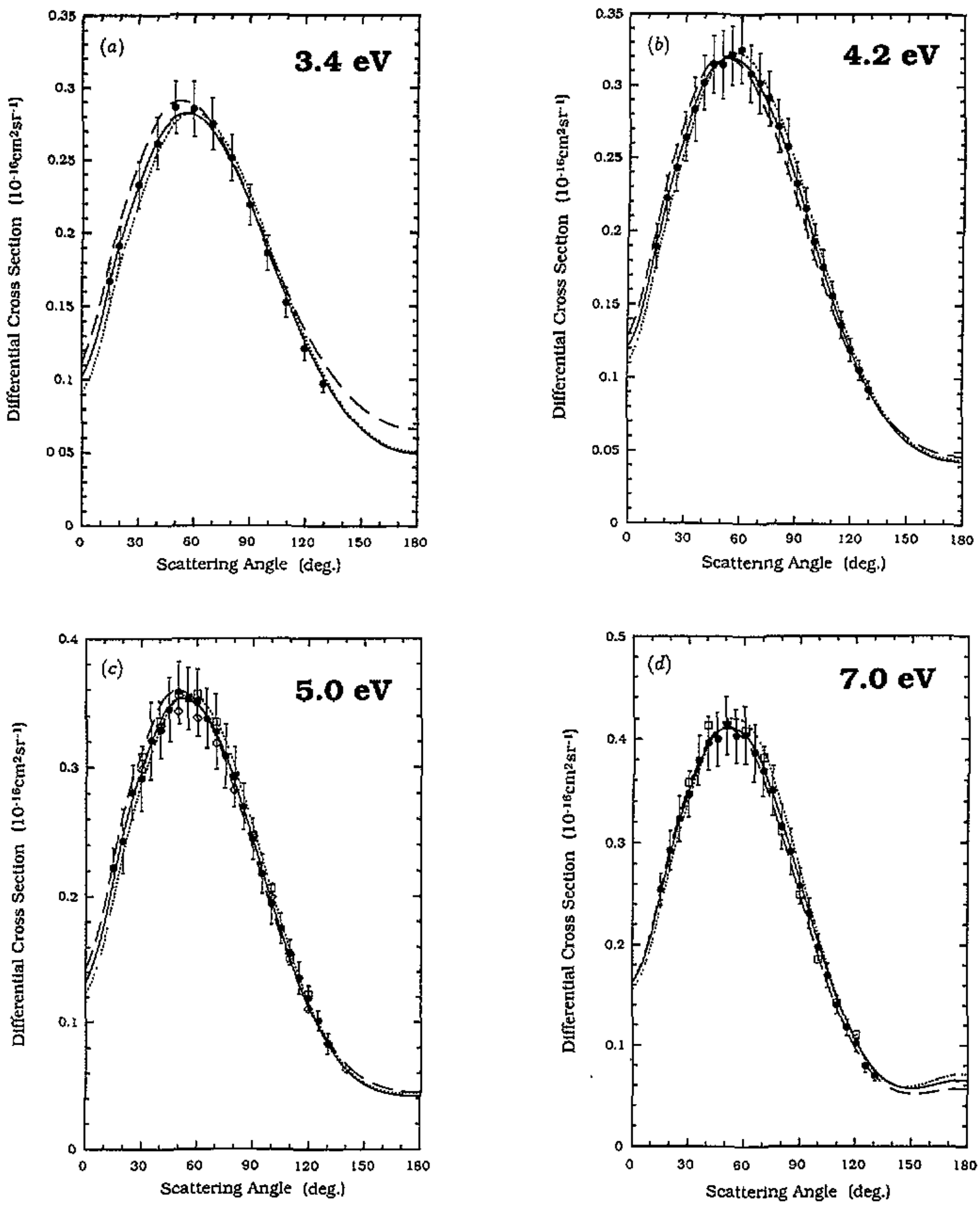

Figure 3. Differential cross sections, in units of 10^{-16} cm^2 sr^{-1}, for electron scattering from neon at (*a*) 3.4 eV, (*b*) 4.2 eV, (*c*) 5.0 eV and (*d*) 7.0 eV: (●) present results; (□) Shi and Burrow; (— —) Williams; (- - -) O'Malley and Crompton; (◇) Register *et al*; (-----) McEachran and Stauffer; (——) Saha.

and to a slightly lesser extent with the cross section of Williams and that of McEachran and Stauffer.

Finally at 7 eV (figure 3(*d*)) we once again see an excellent level of agreement between the present cross section, the theory of Saha, and the measured values of both Williams and Shi and Burrow, at all scattering angles. There is a slight difference in shape between all of the above and the AE polarization calculation of McEachran and Stauffer.

4. Phaseshift analysis

Both the total and differential cross sections have been analysed to extract scattering phaseshifts which can be compared with one another and with other data in the literature.

4.1. Total cross section

In the case of the total cross section the phaseshift analysis has been carried out with modified effective range theory (MERT). MERT has been applied extensively in the analysis and interpretation of low-energy electron scattering by spherically symmetric systems (see, for example, O'Malley 1963, Golden 1966, O'Malley and Crompton 1980, Ferch *et al* 1985, Buckman and Mitroy 1989, Brennan and Ness 1993). A detailed discussion of the applicability of various forms of MERT to the rare gases has been given by Buckman and Mitroy (1989).

The present total cross section for neon has been analysed using a five-parameter version of MERT (MERT5; Buckman and Mitroy). The scattering phaseshifts are expanded in the following fashion

$$\tan \eta_0 = -Ak[1+(4\alpha_d/3)k^2 \ln k] - (\pi\alpha_d/3)k^2 + Dk^3 + Fk^4 \tag{1}$$

$$\tan \eta_1 = a_1\alpha_d k^2 - A_1 k^3 + (b_1\alpha_d^2 + c_1\alpha_q)k^4 + Hk^5 \tag{2}$$

$$\tan \eta_l = a_l\alpha_d k^2 + (b_l\alpha_d^2 + c_l\alpha_q)k^4 \qquad l \geqslant 2 \tag{3}$$

where l is the angular momentum, η_l the lth-order phaseshift, α_d the static dipole polarizability of the atom and α_q is the effective quadrupole polarizability. A (the scattering length), D, F, A_1 and H are fitting parameters. The coefficients a_l, b_l and c_l are given by

$$a_l = \frac{\pi}{(2l+3)(2l+1)(2l-1)} \tag{4}$$

$$b_l = \frac{\pi[15(2l+1)^4 - 140(2l+1)^2 + 128]}{[(2l+3)(2l+1)(2l-1)]^3(2l+5)(2l-3)} \tag{5}$$

$$c_l = \frac{3a_l}{(2l+5)(2l-3)}. \tag{6}$$

For the present analysis, a value of $2.669a_0^3$ (Dalgarno and Kingston 1960) was used for the dipole polarizability and the effective quadrupole polarizability was taken to be zero (see Buckman and Mitroy 1989).

Previous studies have highlighted the relative insensitivity of the MERT fitting procedure to the neon integral cross sections as a result of the small contribution from p- and d-wave scattering and the resultant weak energy dependence of the cross sections.

For instance, the analysis of O'Malley and Crompton (1980) only involved the parametrization of the s-wave, the p- and d-wave values being fixed to those given by an extended MERT fit to the values of Williams (1979). Given these limitations, and others highlighted by Buckman and Mitroy (1989) for MERT when it is used for neon, the main aims of the present analysis were simply to extract the scattering length and the s-wave phaseshifts from the present total cross section data.

The reliability with which we could expect this to be done was tested by fitting the total cross section of Saha using a MERT5 expansion and comparing the derived scattering length and s-wave phaseshift which result from this fit to the calculated values. For these tests we used a similar energy grid for the total cross section points as is available from the experiment although, given the weak energy dependence of the cross section, this is not of great importance. In particular, the minimum energy used was 0.1 eV and a range of maximum energies between 1.0 and 5 eV were investigated. These studies indicate, for example, that even if the fit is carried out to 5 eV, the derived scattering length is within 0.4% of the calculated value, and the derived s-wave phaseshifts are within ±1% of the calculated values for energies less than 3 eV, rising to about 5% different at 5 eV. An analysis of the p-wave phaseshifts indicates that the MERT5-derived values bear little resemblance to the calculated ones, which is consistent with previous observations of the shortcomings of MERT for neon. However, if an analysis is performed where only the s-wave phaseshift is fitted using a three-parameter expansion (MERT3) and the p- and d-wave phases are taken directly from Saha's published values, the derived s-wave phaseshift is within ±1% over the whole energy range from 0.1 to 5.0 eV. Such a MERT3 analysis, when applied to the present time-of-flight (TOF) total cross section, is therefore expected to provide a reliable means of deriving the scattering length and s-wave phaseshift at energies below 5 eV.

In the analysis of the present total cross section using the MERT5 expansion, a number of variations have been investigated. Firstly, the maximum energy (E_{max}) to which the regular MERT5 expansion has been applied was varied over the range 0.5 to 5.0 eV. Secondly, given the apparent insensitivity of the analysis in determining the correct p-wave phaseshift and also the fact that the polarization formula (equation (3)) gives d-wave phaseshifts which differ from those obtained from theory by more than 5% at the higher energies (above ~3 eV), we have carried out the MERT3 analysis using fixed values for the p- and d-wave phaseshifts from Saha's theory. The results of the analysis, including the values of the scattering length obtained from the various fits, are summarized in table 3, where they are also compared with other results from swarm experiment and theory. Based on the tests outlined above and on those conducted by

Table 3. Scattering length (A) and other parameters derived from various MERT analyses of the present total scattering cross section data, compared with results from both theory and swarm experiments.

	MERT3	MERT5 $E_{max}=1.0$ eV	MERT5 $E_{max}=5.0$ eV	O'Malley and Crompton	Saha
A	0.2065	0.2119	0.2087	0.2135	0.2218
D	3.6382	5.3622	3.6825	3.86	
F	−2.6586	8.5669	−2.6795	−2.656	
H	—	−14.561	2.6797	—	
A_1	—	−3.5727	2.2547	—	

Buckman and Mitroy, our preferred value of the scattering length is that obtained from the MERT5 fit between 0.1 and 1.0 eV—0.2119—which is 0.7% lower than that of O'Malley and Crompton and 4.5% lower than that of Saha. The s-wave phaseshifts derived from the MERT3 fit across the entire energy range of the TOF data are compared with other results in section 5.

4.2. *Differential cross sections*

The differential cross sections have been phaseshift analysed using a similar procedure to that employed by Brunger *et al* (1992), which was based on earlier work by Allen (1986) and Allen and McCarthy (1987). In this procedure the differential cross section is expanded as

$$\sigma(\theta, \boldsymbol{a}) = \left| (2k)^{-1} \sum_{l=0}^{\infty} (2l+1)[S_l(\boldsymbol{a}) - 1] P_l(\cos\theta) \right|^2 \tag{7}$$

where

$$S_l(\boldsymbol{a}) = \exp(2\mathrm{i}\delta_l(\boldsymbol{a})) = \prod_{n=1}^{N} \frac{\lambda^2 - \beta_n^2}{\lambda^2 - \alpha_n^2} \tag{8}$$

and $\delta_l(\boldsymbol{a})$ are the phaseshifts for each partial wave, $\lambda = l + 1/2$ and $\boldsymbol{a} = \{a_n\}$ is the set of all the real and imaginary parts of the $2N$ complex parameters α_n and β_n ($n = 1, 2, \ldots, 2N$). In the analysis the function

$$\chi_1^2 = \frac{1}{M-P} \sum_{i=1}^{M} \frac{\sigma_i - \sigma(\theta_i, \boldsymbol{a})}{(\Delta\sigma_i)^2} \tag{9}$$

is minimized and χ_1^2 should be close to unity if the parametrization of (8) is satisfactory and non-statistical errors are small. In this expression, M is the number of data points, $P = 2N$ for real phaseshifts, σ_i is the measured differential cross section at the scattering angle θ_i and $\Delta\sigma_i$ is the *statistical* error in σ_i. The fitting procedure is regularized by actually minimizing

$$\chi^2 = \chi_1^2 + \gamma \sum_{n=1}^{P} (a_n - a_n^{(0)})^2 \tag{10}$$

where the *a priori* information for $\{a_n^{(0)}\}$ is taken from the theory of Saha (1989, 1990). The regularization parameter γ is used to vary the weighting that is given to the *a priori* scattering information. The details of the procedure are discussed in Allen (1986) and Allen and McCarthy (1987). We expect that this approach should prove particularly appropriate for neon where the low-energy differential cross sections show only small angular variations. A similar constrained phase analysis was carried out on neon by Register and Trajmar, although they used the total cross section as the overall constraint.

The results of this analysis, i.e. the phaseshifts at each of the experimental energies used, are shown in table 4. The phaseshifts can also be used to generate total and momentum transfer cross sections with well defined uncertainties and these values are also shown in table 4 and plotted in figures 1 and 4 respectively. The present s-wave phaseshifts are generally in excellent agreement (±1–2%) with those calculated by Saha and McEachran and Stauffer and derived by O'Malley and Crompton, across the entire energy range. The agreement with the s-wave phaseshifts of Williams is similar at all but the lowest energy, where one notices the largest discrepancies between the differential cross section. For the p-wave phaseshifts, large discrepancies occur between all of the above between 1 and 2 eV where the phaseshift changes sign but, as the phaseshift is very small, this does not manifest itself greatly in the DCS. Above 2 eV, there is generally good agreement (±10%) between the present p-wave phaseshifts and all of the above. One exception is the values of McEachran and Stauffer which lie about 20% lower than the others at mid energies (2–3.4 eV). The present d-wave phaseshifts are within ±5–10% of those of O'Malley and Crompton and Saha over most of the common energy range. The values of Williams are systematically lower than the present by 10–50%, the largest differences occurring at the lowest energies, whilst those of McEachran and Stauffer are 5–15% higher than the present across the common energy range.

As may be expected from the level of agreement shown in the differential cross sections and phaseshifts, the present DCS-derived total (figure 1) and momentum transfer (figure 4) cross sections are in excellent agreement (±2%) with those of Saha at all energies up to 7 eV. Below about 3 eV these total cross section values are also in excellent agreement with the present TOF cross section. At higher energies the DCS-derived results show a similar, if slightly less pronounced, difference from the TOF cross section as with the theoretical cross section. At 5 eV the present DCS-derived result, which has an uncertainty of ±5%, lies about 5% below the TOF value. This will be discussed further in the next section.

In figure 4 we also show the momentum transfer cross section of Robertson (1972) which was derived from drift velocity measurements (the same data used by O'Malley and Crompton for their MERT analysis), and the calculated values of McEachran and Stauffer. It is interesting to note that there are similar differences at higher energies in the momentum transfer cross section as seen in the total cross section (figure 1(*b*)). Both the swarm-derived cross section and that of McEachran and Stauffer are higher than the theory of Saha and the present Q_m. In the case of the calculation of McEachran and Stauffer this is a reflection of the slight 'shift' observed in the DCS and commented upon above.

Another interesting aspect of the phaseshift analysis is that in the case of elastic scattering below the first inelastic threshold the analysis can, in principle, be used as an independent means to establish the absolute magnitude of the differential scattering cross section (see for example Andrick and Bitsch 1975, Steph *et al* 1979, Register *et al* 1980). This is generally true when the phaseshifts are real, as they are at energies below the first excited state threshold, and when there is sufficient structure in the angular distribution to enable a unique determination of the several dominant phases which are interfering to cause the observed structure. This in turn requires the energy to be high enough so that there is more than one scattering phase contributing to the shape of the elastic angular distribution, but low enough that there are not too many such phases interfering with one another. The present analysis is capable of such a determination by introducing an additional renormalization parameter κ in equation (9) which then becomes

$$\chi_1^2=\frac{1}{M-P}\sum_{i=1}^{M}\frac{\sigma_i-\kappa\sigma(\theta_i,\boldsymbol{a})}{(\Delta\sigma_i)^2} \tag{11}$$

(see Allen and McCarthy 1987). The fits were carried out to the experimentally determined absolute data set at each energy and the values of the renormalization parameters

Table 4. Phaseshifts (in radians), integral cross sections Q_{el} and Q_{mt} (in Å^2), and fitting parameters derived from the present differential cross sections, compared with results from the TOF measurements and those from other experimental and theoretical investigations.

E (eV)	Reference	η_0	η_1	η_2	η_3	K	χ^2	Q_{el}	Q_{mt}
0.75	Present (from DCS)	−0.1493	0.00547	0.00516	0.00130	1.000	0.631	1.43	1.52
	Present TOF (MERT3)	−0.1483	—	—	—			1.41	—
	Williams*	−0.144	0.0018	0.0025	—			1.31	1.34
	O'Malley and Crompton*	−0.147	0.0059	0.0043	—			1.39	1.49
	McEachran and Stauffer	−0.1467	0.00690	0.00452	0.00147			1.38	1.50
	Saha*	−0.1488	0.00566	0.00419	0.00120			1.42	1.51
1.0	Present (from DCS)	−0.1811	0.00298	0.00638	0.00183	0.998	0.477	1.57	1.61
	Present TOF (MERT3)	−0.1821	—	—	—			1.57	—
	Williams*	−0.182	0.00042	0.0040	—			1.57	1.57
	O'Malley and Crompton	−0.181	0.004	0.006	—			1.57	1.62
	McEachran and Stauffer	−0.1800	0.00504	0.00611	0.00196			1.55	1.62
	Saha	−0.1809	0.00383	0.00574	0.00161			1.56	1.62
1.3	Present (from DCS)	−0.2211	−0.00225	0.00770	0.00206	1.000	0.16	1.78	1.75
	Present TOF (MERT3)	−0.2182						1.73*	—
	Williams*	−0.221	−0.0028	0.0057	—			1.78	1.73
	O'Malley and Crompton*	−0.217	−0.0007	0.00770	—			1.73	1.71
	McEachran and Stauffer	−0.2164	0.00134	0.00808	0.00255			1.71	1.73
	Saha*	−0.2175	−0.00075	0.00750	0.00210			1.73	1.71
2.2	Present (from DCS)	−0.3106	−0.0186	0.01315	0.00369	1.000	5.58	2.08	1.85
	Present TOF (MERT3)	−0.3130	—	—	—			2.13*	—
	Williams*	−0.314	−0.0192	0.0112	—			2.11	1.87
	O'Malley and Crompton[1]	−0.3100	−0.0190	0.0130	—			2.09	1.86
	McEachran and Stauffer*	−0.3098	−0.0161	0.0144	0.00434			2.07	1.87
	Saha*	−0.3102	−0.0187	0.0131	0.00369			2.07	1.85

Table 4. (continued)

E (eV)	Reference	η_0	η_1	η_2	η_3	K	χ^2	Q_{el}	Q_{mt}
3.4	Present (from DCS)	−0.4090	−0.0507	0.0228	0.0065	1.018	0.82	2.38	1.90
	Present TOF (MERT3)	−0.4226	—	—	—			2.53*	—
	Williams	−0.413	−0.048	0.018	—			2.49	2.03
	McEachran and Stauffer*	−0.4132	−0.04577	0.0237	0.00675			2.41	1.97
	Saha	−0.4118	−0.0482	0.0215	0.0063			2.39	1.93
4.2	Present (from DCS)	−0.4709	−0.0689	0.0283	0.00796	1.000	0.62	2.56	1.97
	Present TOF (MERT3)	−0.4696	—	—	—			2.74*	—
	Williams*	−0.469	−0.069	0.023	—			2.53	1.93
	McEachran and Stauffer*	−0.4765	−0.0672	0.0306	0.00839			2.61	2.04
	Saha*	−0.4716	−0.0690	0.0275	0.00777			2.57	1.98
5.0	Present (from DCS)	−0.5297	−0.0891	0.0327	0.00898	1.000	0.22	2.73	2.04
	Present TOF (MERT3)	−0.5542	—	—	—			2.89	—
	Robertson							—	2.07
	Williams*	−0.529	−0.091	0.029	—			2.73	2.01
	Register and Trajmar	−0.5220	−0.0911	0.0344	0.00698			2.68	1.99
	McEachran and Stauffer	−0.5300	−0.0898	0.0379	0.0101			2.76	2.07
	Saha	−0.5254	−0.0913	0.0340	0.00940			2.71	2.01
7.0	Present (from DCS)	−0.6442	−0.1413	0.0520	0.0131			2.98	2.13
	Robertson							—	2.21
	Williams*	−0.637	−0.143	0.047	—			2.92	2.05
	McEachran and Stauffer*	−0.6525	−0.1437	0.0580	0.0144			3.07	2.21
	Saha*	−0.6495	−0.1407	0.0516	0.0129			3.01	2.16

* Indicates interpolated value(s).

[1] Values for their highest energy of 2.176 eV.

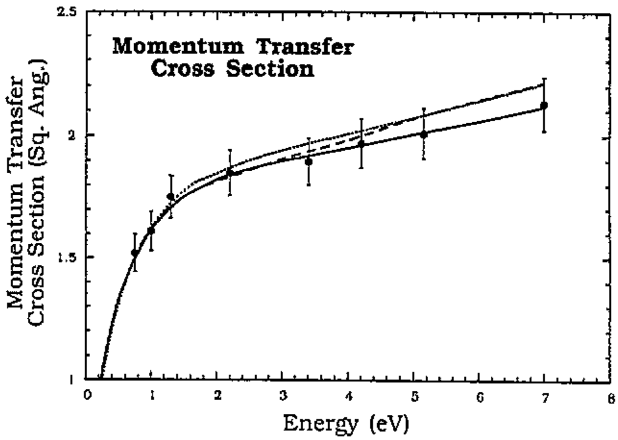

Figure 4. Momentum transfer cross section in units of Å^2 for electron scattering from neon: (•) present results; (- - -) Robertson; (-----) McEachran and Stauffer; (——) Saha.

are also given in table 4. These indicate that there is excellent agreement between the absolute scale determined as a result of the *shape* of the angular distribution and that established with the relative flow technique.

5. Discussion and conclusions

The present results for both differential and total scattering clearly add to the high level of agreement that exists between a substantial number of experimental and theoretical investigations of low-energy electron scattering from neon. This is particularly true at energies below 2 eV where there has been uncertainty due to discrepancies between recent and past experimental differential cross section measurements. This excellent agreement between experiment and *ab initio* scattering theory now exists at a number of different levels in the hierarchy of scattering cross sections, from total and swarm-derived momentum transfer cross sections to differential cross sections, and to the phaseshifts derived from all of these measurements using various techniques.

At higher energies the picture is not quite so clear, the principal problem arising from the differences between the integral cross sections, particularly the most recent total cross sections of Nickel *et al* (1984), Kumar *et al* (1987), the present TOF measurements, those derived from the present DCS measurements and also those from the various theories. These differences, of up to 6%, are outside what one would expect given the level of agreement observed in the differential cross sections, and given the high accuracy expected from the 'direct' total scattering measurements. Similar differences are observed in the momentum transfer cross section where the cross section of Robertson slowly departs from the theory of Saha at energies above 3 eV. Whilst it could be argued that the swarm-derived result may be less accurate at these higher energies no such arguments can be raised against the attenuation measurements, particularly in the case of neon where the elastic differential cross sections are not forward peaked and the cross sections are relatively small. It is also most unlikely that the differences in the total cross section can be due to either an error in the energy scale or the absolute calibration of the spinning rotor gauge. In the first case the uncertainty in the energy scale which arises from the TOF calibration is at most −150 meV at 5 eV, and as the cross section varies only slowly with energy this cannot be responsible for the observed differences. In the second case, an error in the absolute pressure calibration might be expected to manifest itself at all energies and not just at the higher end of the present measurement range.

As a result of these differences in the total cross section at higher energies, we performed a number of separate, comparative measurements with the TOF apparatus, under *identical* electron-optical operating conditions and for a variety of gas pressures, of the total cross sections for N_2, He and Ne at an energy of 5 eV. These results were compared with the measurements of Kennerly (1980) and Nickel *et al* (1992) for N_2 and with the measurement of Jones and Bonham (1982) and the theory of Nesbet (1979) for He. The N_2 cross section of 11.85 Å^2 which was obtained from these measurements is 2.1% higher than that of Kennerly and 1.2% lower than Nickel *et al.* The He cross section of 5.34 Å^2 is identical to that of Jones and Bonham and 0.6% lower than that of Nesbet. Whilst this good agreement is not conclusive, it does provide further support for the accuracy of the neon total cross section measurements as it is difficult to imagine any gas-specific effects which could result in the overestimation of the neon cross section alone.

These differences are hard to reconcile and pose a dilemma in supporting the use of neon as a secondary scattering 'standard', at the ±2–3% level, at energies above about 3 eV. It is somewhat unusual that in this case the disagreement occurs at the level of the integral cross section, whilst the best agreement within and between experiment and theory comes at the level of the differential cross section. Given the low energies involved and the small magnitude of the cross section, one may have intuitively expected the reverse situation to be more likely. Indeed, one generally considers the total cross section as the first-order test of experiment and theory because, whilst it is less sensitive to the dynamics of the scattering process, the level of accuracy with which it can (supposedly) be measured makes it an important tool in the comparison process.

In summary, given the agreement between experiment and theory at the level of the differential cross section, one would have little hesitation in concluding that the neon elastic scattering cross section is well understood at energies below 10 eV, and that the phaseshifts that result from the multiconfiguration Hartree–Fock calculation of Saha (1989, 1990) provide cross sections which are generally in excellent agreement with a number of recent measurements, including the present data set. Consequently one is compelled, despite the apparent lack of corroboration from the present total cross section results at higher energies, to suggest that these calculated phaseshifts give a good representation of the scattering process, at least at the 5% level, and thus qualify neon in the role as a secondary elastic scattering cross section 'standard'. Certainly it appears that measurements of the elastic cross section in neon, in conjunction with the relative flow technique and the use of helium as a cross section standard, could well be used as a check of the operation of any low-energy electron spectrometer. In addition, given the small absolute value of the cross sections involved, particularly at forward scattering angles, such measurements also provide a rigorous test of electron optics and the optimization of signal/noise conditions.

The data presented here are typical of many other experiments in the literature, which claim high accuracy and which appear to be based on sound experimental practice, yet which disagree with one another outside the claimed uncertainties for common scattering processes. Perhaps the scattering community does not yet fully understand the wide range of possible systematic errors that can affect such measurements.

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