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The scattering of low-energy electrons by argon atoms

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Abstract. Phaseshifts, differential, total and momentum transfer cross sections are calculated using an R-matrix approach for the elastic scattering of electrons by argon atoms in the impact energy range 0–19 eV. The coupled-state calculation is based upon a single-configuration atomic ground-state wavefunction coupled to a ^{1}P pseudostate. A critical assessment of earlier theoretical and experimental data is made and the conclusion is reached that the present results are the most satisfactory over the entire energy range considered.

1. Introduction

For almost two decades, the scattering of low-energy electrons by argon atoms has received considerable theoretical and experimental study. A wealth of data has been produced for total elastic and momentum transfer cross sections and for differential cross sections (see Fon *et al* 1983, McEachran and Stauffer 1983 and references therein). However, considerable disagreement still exists between different sets of experimental data, between different theoretical treatments and between theory and experiment.

In this paper we restrict our attention to the impact energy range 0–19 eV; in this range the two most interesting features in total elastic and momentum transfer cross sections appear; namely, the Ramsauer–Townsend minimum and the maximum due to the d-wave resonance. Particular attention is paid to the phaseshifts since the work is partly motivated by the need for accurate free–free absorption and bremsstrahlung cross sections. The phaseshifts may be used either as a means of assessing the accuracy of an *a priori* calculation of these quantities or to actually calculate them using approximate formulae such as those derived by Ritchie (1981) or John *et al* (1974).

The most recent theoretical calculations in this energy range are those by McEachran and Stauffer (1983), Fon *et al* (1983) and Amusia *et al* (1982). McEachran and Stauffer employed a polarised-orbital approximation which included both polarisation and exchange potentials. However they did not include the polarised exchange terms which arise naturally in their theory and which could be of significance at these low energies. Amusia *et al* used many-body perturbation theory and the simplified random-phase approximation with exchange to obtain an optical potential. Fon *et al* employed an R-matrix approach in which polarisation and exchange were included by coupling a ^{1}P pseudostate to the argon ground state. Their calculation however excluded the region of the Ramsauer–Townsend minimum and was performed for impact energies greater than 3 eV.

2. Theory

In this paper an R-matrix approach is also adopted and the calculations were performed using the R-matrix program described by Berrington *et al* (1978). We assume that the effects of spin–orbit coupling and other relativistic effects may be neglected and that the calculation may be performed in LS coupling. Two states of the argon atom were included in the eigenfunction expansion. The ground state of argon was represented by the single-configuration Hartree–Fock wavefunction obtained by Clementi and Roetti (1974). A ^{1}P pseudostate was added to this (to allow for the ground-state static dipole polarisability) and this ^{1}P state was represented by a linear combination of three configurations, namely $3s^2\,3p^5\,\overline{3d}$, $3s^2\,3p^5\,\overline{4s}$ and $3s^2\,3p^5\,\overline{4d}$.

For both atomic states the one-electron radial orbitals are expressed in the form

$$P_{nl}(r) = \sum_i c_i r^{p_i} \exp(-\xi_i r)$$

and for 1s, 2s, 2p, 3s and 3p the parameters c_i, p_i and ξ_i were taken from Clementi and Roetti (1974). These parameters for the remaining $\overline{3d}$, $\overline{4s}$ and $\overline{4d}$ pseudo-orbitals occurring in the ^{1}P pseudostate were determined by optimising the ground-state static dipole polarisability following Vo Ky Lan *et al* (1976) using the code CIVPOL with the single-configuration ground state and the ^{1}P pseudostate described above.

The value obtained for the static dipole polarisability was $12.57a_0^3$. The experimental value, from the recommendation of Miller and Bederson (1977), is $11.1a_0^3$. We note that the present ^{1}P pseudostate differs from that used by Fon *et al* (1983): in particular, by the omission of a $\overline{4p}$ pseudo-orbital. This orbital entails opening the 3s subshell which gives rise to an inordinately large number of $(N+1)$ electron correlation orbitals. Its exclusion has only a small effect as can be seen from the value of $12.79a_0^3$ calculated by Fon *et al* for the static dipole polarisability.

The R-matrix program was then utilised by including six continuum orbitals for each incident electron orbital angular momentum $l = 0$, 1, 2, 3 and 4, the R-matrix radius being taken to be 10.2 au.

Unfortunately, the results obtained from the calculation just described turned out to be in serious disagreement with both other theoretical treatments and with experiment. In particular, exceedingly poor values were obtained for the scattering length and for the energies at which the Ramsauer–Townsend minimum occurs in the elastic scattering and momentum transfer cross sections. Attempts were then made at improving the calculation by systematically increasing the degree of sophistication of both the ground state and ^{1}P pseudostate of the argon atom by the inclusion of further configurations. The net result, however, was to reveal no significant improvement or convergence of the scattering length or the Ramsauer–Townsend minimum positions towards those derived experimentally.

Closer examination of these various calculations revealed a remarkable sensitivity of the scattering length and the Ramsauer–Townsend minima to small variations in the position of the lowest-lying R-matrix pole in the ^{2}S symmetry. This pole is strongly coupled to the $3p^6\,\overline{4s}\,^2S$ $(N+1)$ bound state which is included in the eigenfunction expansion for orthogonality reasons.

An alternative method of consistently improving the calculation was therefore adopted. Employing the single-configuration ground state, the ^{1}P pseudostate, the R-matrix boundary and the continuum orbitals as described above for the initial calculation, the R-matrix program was run with the $3p^6\,\overline{4s}\,^2S$ $(N+1)$ bound state shifted in position by the small energy difference of −0.00125 au. This choice of shift was made by adopting that value which produced a scattering length and Ramsauer–Townsend minimum positions in close agreement with those obtained experimentally. The scattering length obtained was $-1.68a_0$ which is in good agreement with the experimentally derived values of $-1.63a_0$ (Gus'kov *et al* 1978) and $-1.65a_0$ (Golden and Bandel 1966) derived from elastic scattering cross section measurements and in fair agreement with that derived by Golovanivsky and Kabilan (1980) ($-1.53a_0$) from momentum transfer cross section data. All of the results presented in the next section were obtained from the $(N+1)$ bound state shifted calculation discussed above and where necessary higher partial-wave contributions were added by employing phaseshifts derived from the effective-range theory of Rosenberg *et al* (1961). In the energy range considered the effective-range theory provides higher partial-wave phaseshifts (Fon *et al* 1983) of adequate accuracy since contributions to the cross sections are in general quite small.

3. Results and discussion

Table 1 contains the present results for the elastic scattering cross section, the momentum transfer cross section and the phaseshifts for incident electron angular momenta $l = 0, 1, 2$ and 3. Before comparing these results with other theoretical and experimental data, the reader's attention is drawn to the fact that figures 1(a), 2(a), 4(a) and 4(b) employ logarithmic scales.

Table 1. Total elastic (Q) and momentum transfer (Q_M) cross sections (in units of πa_0^2) and phaseshifts (η_l) (in radians) for the the elastic scattering of electrons by argon.

E(eV)	Q	Q_M	η_0	η_1	η_2	η_3
0.02	5.41	4.65	4.426^{-2}	3.092^{-3}	5.836^{-4}	1.537^{-4}
0.06	2.80	1.96	5.363^{-2}	8.155^{-3}	1.577^{-3}	5.210^{-4}
0.1	1.70	9.38^{-1}	5.133^{-2}	1.219^{-2}	2.686^{-3}	8.937^{-4}
0.2	6.43^{-1}†	1.64^{-1}	3.255^{-2}	1.930^{-2}	5.516^{-3}	1.831^{-3}
0.3	3.81^{-1}	1.36^{-1}	8.595^{-3}	2.307^{-2}	8.379^{-3}	2.756^{-3}
0.4	3.89^{-1}	3.03^{-1}	-1.639^{-2}	2.460^{-2}	1.128^{-2}	3.667^{-3}
0.5	5.13^{-1}	5.25^{-1}	-4.122^{-2}	2.444^{-2}	1.419^{-2}	4.574^{-3}
0.7	9.06^{-1}	9.81^{-1}	-8.931^{-2}	2.040^{-2}	2.016^{-2}	6.374^{-3}
1.0	1.61	1.59	-1.566^{-1}	8.199^{-3}	2.927^{-2}	9.059^{-3}
2.0	4.08	3.23	-3.480^{-1}	-5.612^{-3}	6.446^{-2}	1.788^{-2}
3.0	6.46	4.93	-5.057^{-1}	-1.329^{-1}	1.111^{-1}	2.669^{-2}
5.0	1.09^{1}	8.77	-7.575^{-1}	-2.901^{-1}	2.316^{-1}	4.534^{-2}
6.0	1.30^{1}	1.07^{1}	-8.610^{-1}	-3.644^{-1}	3.017^{-1}	5.522^{-2}
7.0	1.50^{1}	1.25^{1}	-9.539^{-1}	-4.336^{-1}	3.810^{-1}	6.523^{-2}
8.0	1.70^{1}	1.41^{1}	−1.038	-4.971^{-1}	4.695^{-1}	7.529^{-2}
9.0	1.90^{1}	1.54^{1}	−1.116	-5.546^{-1}	5.641^{-1}	8.549^{-2}
10.0	2.07^{1}	1.63^{1}	−1.186	-6.063^{-1}	6.610^{-1}	9.600^{-2}
12.0	2.34^{1}	1.69^{1}	−1.311	-6.940^{-1}	8.575^{-1}	1.186^{-1}
14.0	2.48^{1}	1.62^{1}	−1.420	-7.641^{-1}	1.055	1.438^{-1}
16.0	2.48^{1}	1.47^{1}	−1.521	-8.197^{-1}	1.223	1.736^{-1}
18.0	2.37^{1}	1.30^{1}	−1.585	-1.550^{-1}	1.342	2.132^{-1}
19.0	2.32^{1}	1.22^{1}	−1.612	-8.700^{-1}	1.388	2.422^{-1}

† The superscript denotes the power of 10 by which the number is to be multiplied.

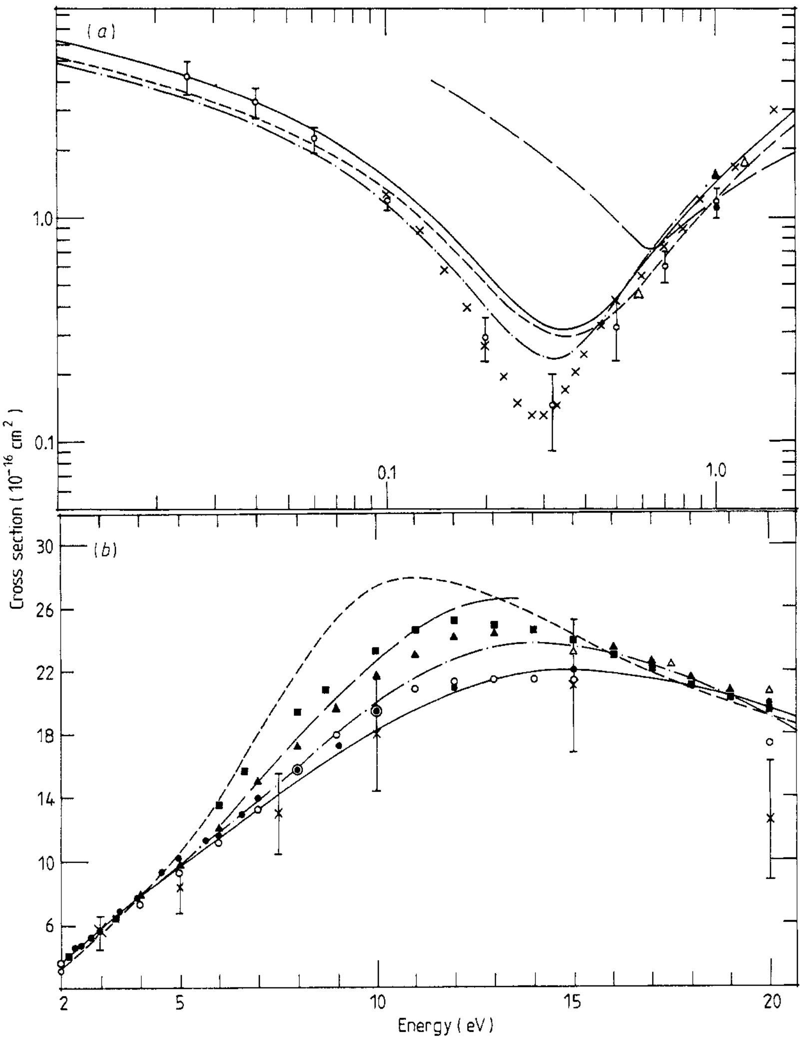

Figure 1. Elastic scattering cross section. (a) Theory: ——, present results; - - - -, McEachran and Stauffer (1983); – –, Amusia *et al* (1982). Experiment: ▲, Andrick and Bitsch (1984); – · –, Haddad and O'Malley (1982); △, Williams (1979); $\overline{\underline{\circ}}$, Gus'kov *et al* (1978); ●, Kauppila *et al* (1976); ×, Golden and Bandel (1966). (b) Theory: ——, present results: – · –, Fon *et al* (1983); - - - -, McEachran and Stauffer (1983); – –, Amusia *et al* (1982). Experiment: ▲, Andrick and Bitsch (1984); ×, Srivastava *et al* (1981); ●, Charlton *et al* (1980); △, Wagenaar and de Heer (1980); ○, Kauppila *et al* (1976, 1981); ■, Williams (1979).

Figure 1(a) compares the elastic scattering cross section results with the most recent theoretical calculations and with experiment. The data of Haddad and O'Malley (1982) have been derived from a phaseshift analysis of the experimental data for the momentum transfer cross section obtained by Milloy *et al* (1977). Clearly the values of Amusia *et al* (1982) are in severe disagreement with all of the other results. The present results are in close agreement with those of McEachran and Stauffer (1983) but both sets of data fail to give the depth of the Ramsauer–Townsend minimum. At energies away from the minimum highly satisfactory accord is found between the present results and experiment.

Figure 1(*b*) compares the present results with other available data at the higher impact energies. The most noticeable feature is the disagreement between the experimental results. The data of Andrick and Bitsch (1984), Srivastava *et al* (1981) and Williams (1979) have been obtained from differential cross section measurements whereas those of Charlton *et al* (1980), Wagenaar and de Heer (1980) and Kauppila *et al* (1976, 1981) are from direct measurements. The present results are in best agreement with those obtained by direct measurement and in astonishingly good

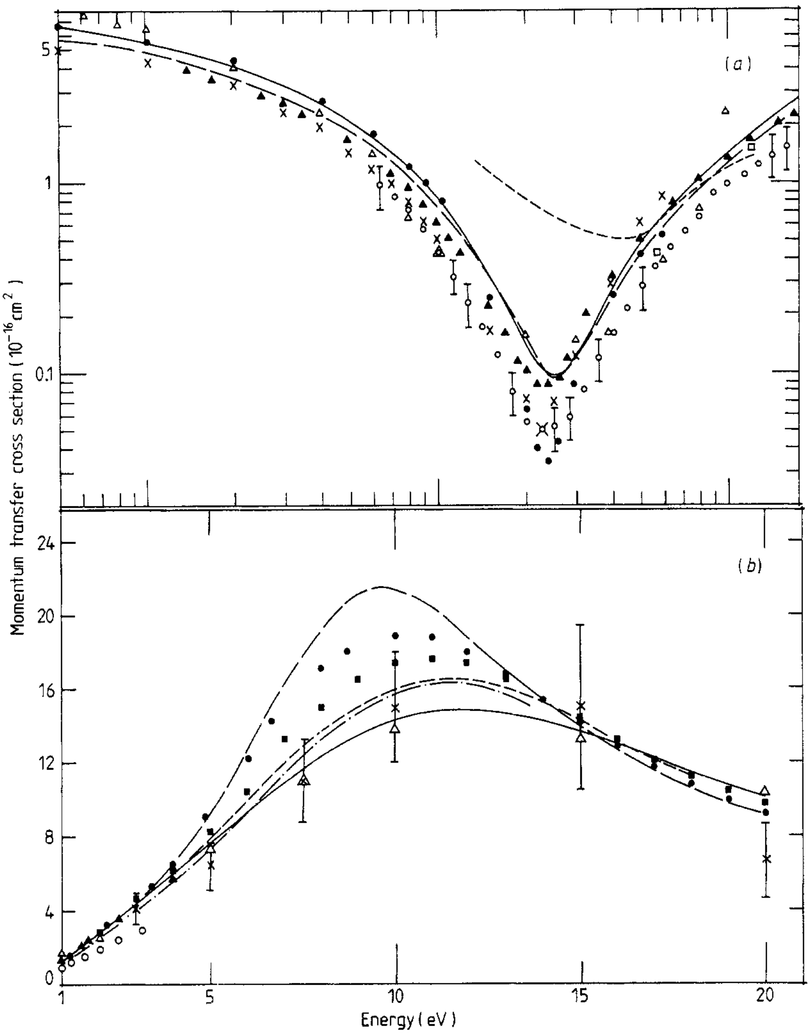

Figure 2. Momentum transfer cross section. (*a*) Theory: ——, present results; – –, McEachran and Stauffer (1983); - - - -, Amusia *et al* (1982). Experiment: ×, Golovanivsky and Kabilan (1980); □, Williams (1979); ▲, Milloy *et al* (1977); ○, McPherson *et al* (1976); ●, Golden (1966); △, Frost and Phelps (1964). (*b*) Theory: ——, present results; - - - -, Fon *et al* (1983); – –, McEachran and Stauffer (1983); – · –, Amusia *et al* (1982). Experiment: ■, Andrick and Bitsch (1984); $\bar{\underline{\text{x}}}$, Srivastava *et al* (1981); ●, Williams (1979); ▲, Milloy *et al* (1977); ○, McPherson *et al* (1976); △, Frost and Phelps (1964).

agreement with the data of Charlton *et al* (1980), who claimed an accuracy of better than 4%.

Figure 2(a) and (b) make similar comparisons for the momentum transfer cross section. Again the present results lie close to those obtained by McEachran and Stauffer (1983) at low impact energies and both are in good agreement with experiment away from the minimum. At the minimum they are also in good agreement with the data of Milloy *et al* (1977) who do not find the same depth as found by Golovanivsky and Kabilan (1980), McPherson *et al* (1976) and Golden (1966). At higher impact energies around the maximum one again finds disagreement between differential and direct cross section experimental data. The present results again lie in remarkable agreement with the only direct measurement (Frost and Phelps 1964).

In order to further analyse the results, figure 3 presents the $l=0$, 1 and 2 phaseshifts. For clarity the $l=0$ and 1 phaseshifts obtained by McEachran and Stauffer (1983) and Fon *et al* (1983) for $k \geqslant 0.25$ au are not shown. The data of McEachran and Stauffer (1983) for these cases lie close to the data of Williams (1979) and the results of Fon *et al* (1983) lie between the present results and those of McEachran and Stauffer. Highly satisfactory agreement exists between theory and experiment for all cases with two exceptions—the $l=1$ phaseshift for $k \leqslant 0.25$ and the $l=2$ phaseshift for $k \geqslant 0.5$.

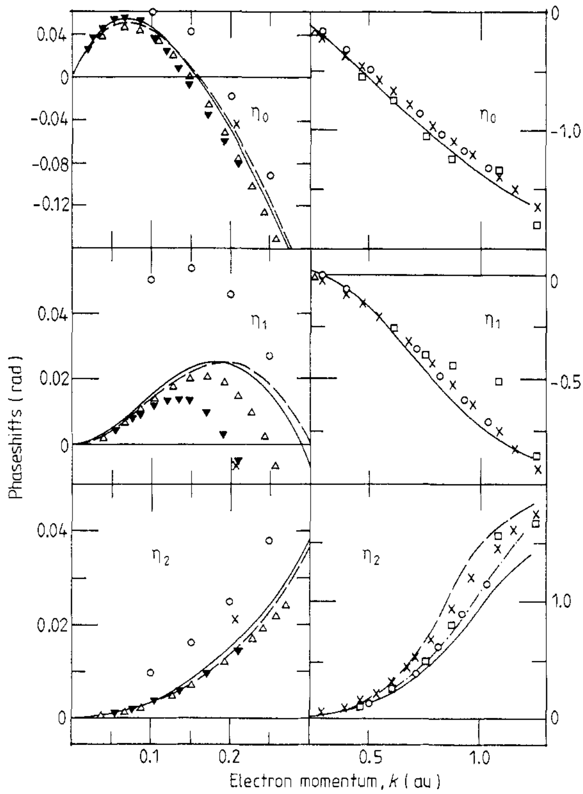

Figure 3. Phaseshifts for elastic scattering of electrons by argon. Theory: ——, present results; - · -, Fon *et al* (1983); - -, McEachran and Stauffer (1983); ○, Amusia *et al* (1982). Experiment: △, Haddad and O'Malley (1982); □, Srivastava *et al* (1981); ×, Williams (1979); ▼, Golden (1966).

These two cases are of course directly connected with the position and depth of the Ramsauer–Townsend minima and with the d-wave maxima and the discrepancies in the phaseshifts are directly related to the varying results discussed above for total elastic and momentum transfer cross sections. Neither the present results nor the values obtained by McEachran and Stauffer (1983) lie close to experiment for the $l=1$, $k \leq 0.25$ phaseshifts. Clearly further work is desirable since figure 3 reveals considerable discrepancy between the phaseshifts derived by Haddad and O'Malley (1982) from the momentum transfer cross section data of Milloy *et al* (1977) and those obtained from total cross sections (Golden 1966) and differential cross sections (Williams 1979).

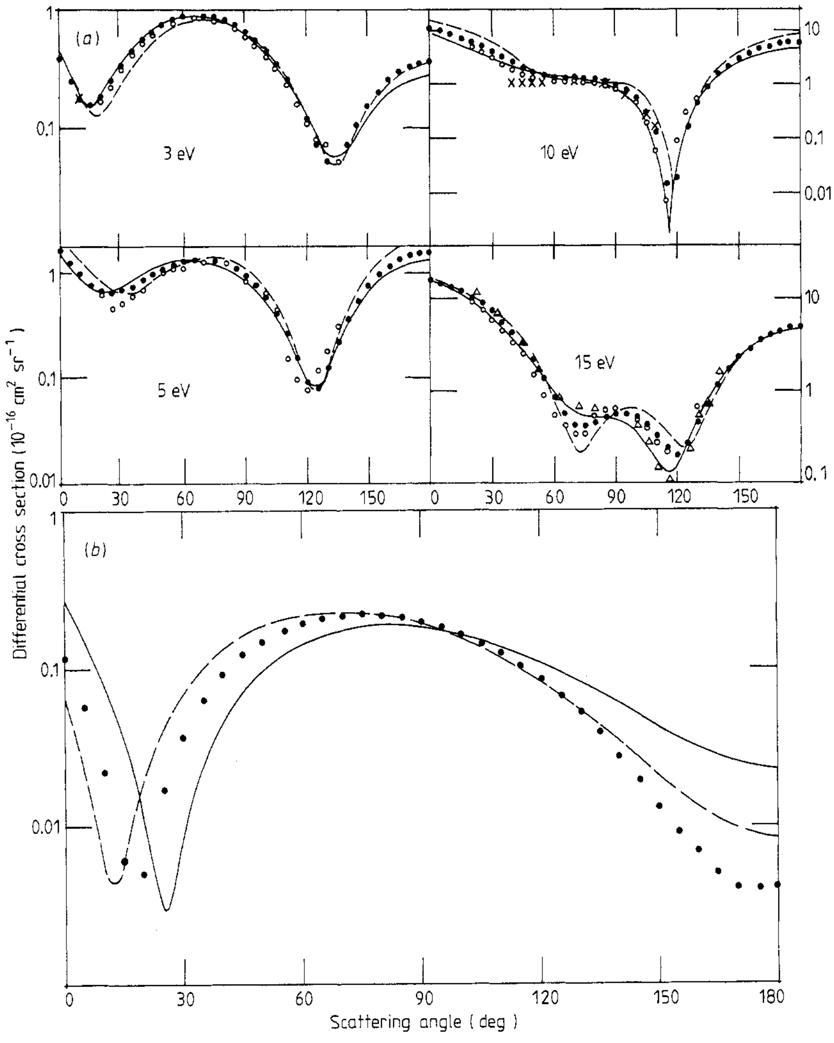

Figure 4. (*a*) Differential cross sections for elastic scattering of 3, 5, 10 and 15 eV electrons by argon. Theory: ——, present results; – –, McEachran and Stauffer (1983). Experiment: ●, Andrick and Bitsch (1984); ×, Zhou Qing *et al* (1982); ○, Srivastava *et al* (1981); △, Lewis *et al* (1974). (*b*) Differential cross section for elastic scattering of 1 eV electrons by argon. Theory: ——, present results. Experiment: ●, Andrick and Bitsch (1984); – –, Haddad and O'Malley (1982).

For the $l=2$, $k \geqslant 0.5$ phaseshifts the only experimental data are those derived from differential cross section measurements. The present results lie lower than those experimental values and also lower than previous theoretical values.

Finally figures 4(*a*) and (*b*) compare differential cross section data for impact energies 3, 5, 10, 15 eV and 1 eV respectively. At 3, 5 and 10 eV, the present results are in good agreement with experiment and at 10 eV in particular where a sharp minimum occurs at about 115°. Attention however should be drawn to the differential cross section at 15 eV. The calculations of McEachran and Stauffer (1983) and of Fon *et al* (1983) (not shown in figure 4(*a*)) both show distinct double minima in agreement with the experimental data of Andrick and Bitsch (1984) and Srivastava *et al* (1981). The present results do not show similar behaviour and are in close accord with the experimental measurement of Lewis *et al* (1974). Figure 4(*b*), which displays the differential cross section at 1 eV, is simply included to reveal the sensitivity of this cross section to the $l=1$ phaseshift. The discrepancies in the phaseshifts displayed in figure 3 manifest themselves quite clearly in figure 4(*b*), particularly in the minimum in the forward direction and also in the backward scattering cross section.

4. Conclusion

Consideration of the differential, total elastic and momentum transfer cross sections together with phaseshift analysis indicates that the present phaseshifts are currently the most satisfactory over the impact energy range 0–19 eV. An exception to this conclusion is the inaccuracy of the $l=1$ phaseshift over the momentum range $k \simeq 0.15$ to $k=0.3$. The phaseshifts should therefore be useful for other purposes such as the calculation of free–free absorption cross sections. A number of discrepancies and areas of disagreement, not only between theoretical work but also between experimental data have been highlighted and further work is clearly desirable.

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