

Differential cross sections and Stokes parameters for electron-magnesium scattering

J Mitroy and I E McCarthy

School of Physical Sciences, The Flinders University of South Australia, Bedford Park, SA 5042, Australia

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Abstract. Differential cross sections and Stokes parameters are reported for electron-magnesium scattering computed in the coupled-channels approximation. A configuration interaction representation is used for the five lowest singlet states which are included in the close-coupling expansion. The calculated differential cross sections for elastic scattering and the resonance $(3s^2)^1S^e-(3s3p)^1P^o$ transition are in fair accord with experimental data, as are total cross sections for the resonance transition. There are only minor discrepancies in the comparison of the computed Stokes parameters with experiment.

1. Introduction

The calculation of electron-atom scattering at energies well above the lower excitation thresholds has a long way to go before results can be obtained within experimental error for absolute cross sections. A striking example is sodium (Mitroy *et al* 1987), where calculated differential cross sections at larger angles can differ from experiment by an order of magnitude. The elastic and the first dipole excitation channels provide a good preliminary test. The dipole excitation yields a diversity of data in the form of m -dependent ratios, which can be expressed as Stokes parameters.

A good idea of the order of magnitude of the difficulties to be encountered in the case of a particular target can be obtained by a coupled-channels calculation. The interaction is dominated by long-range dipole couplings, so it is necessary to include at least the lowest channels that have dipole coupling with the elastic and resonant channels. In the case of magnesium the simplest calculation with these features couples the following channels $(3s^2)^1S^e$, $(3s3p)^1P^o$, $(3s4s)^1S^e$, $(3s3d)^1D^e$, $(3s4p)^1P^o$. This calculation is reported here for incident energies of 10, 20, 40 and 100 eV.

There have been a number of experimental and theoretical investigations of the electron-magnesium reaction. Robb (1974) used the first Born approximation (with configuration interaction wavefunctions) to compute the generalised oscillator strength (GOS) and total cross section for the $(3s^2)^1S^e-(3s3p)^1P^o$ resonant transition. These results were used to put the optical emission excitation functions of Leep and Gallagher (1976) on an absolute scale. Differential cross sections for elastic scattering and inelastic scattering to the resonant first excited state (and a number of other states) have been measured by Williams and Trajmar (1978) at incident energies of 10, 20 and 40 eV. These cross sections were normalised to an absolute scale by the GOS technique and have a relatively low absolute accuracy. Apart from the first Born calculation of Robb (1974), there has also been a two-state close-coupling calculation by Fabrikant (1980),

an optical potential calculation by Khare *et al* (1983), and a first-order many-body theory (FOMBT) calculation by Meneses *et al* (1987).

More recently, Brunger *et al* (1988a) have reported differential cross sections for the resonant excitation with greatly improved error tolerances. Brunger *et al* (1988b) have also reported Stokes parameters for the resonant transition for small-angle scattering at low energies. While the calculations mentioned above provide an adequate description of the experimental data of Williams and Trajmar (1978), the new experiments of Brunger *et al*, with their much more stringent error bounds, show the inadequacies of these earlier calculations.

In the present work we report the results of close-coupling calculations of electron-magnesium scattering at a number of energies above the ionisation threshold. While it might be expected that electron-magnesium scattering would have a number of similarities with electron-helium scattering, this is only superficially true. The large oscillator strength (~ 1.8) and small energy difference between the $(3s^2)^1S^e$ and $(3s3p)^1P^o$ states will cause the coupling between these two levels to be very strong. In this respect the reaction dynamics of the electron-magnesium system is similar to that of the electron-sodium system which is dominated by the coupling of the 3s and 3p levels. In one important respect magnesium is different from sodium. The sodium atom, consisting of a loosely-bound valence electron outside a tightly-bound neon-like core, can be adequately represented by single-configuration Hartree-Fock (HF) wavefunctions. Such a description is not appropriate for the magnesium target states, which should be represented by configuration interaction (CI) wavefunctions (Weiss 1967) in which correlations between the two valence electrons are included. In the calculations reported in this work we have neglected triplet target states, the higher singlet states and the ionisation channels.

Comparison of electron-sodium and electron-magnesium scattering is of more than incidental value. In a previous detailed analysis of electron-sodium scattering (Mitroy *et al* 1987) large differences between all of the calculations and the experimental data on large-angle elastic scattering for neon and sodium were an indication that it was the experiment, and not the theory, that was deficient in some respect. Accordingly, it would be interesting to compare backward angle elastic cross sections at high energies.

2. Details of the calculation

It is well known that the Hartree-Fock (HF) model does not provide a good description of the ground and excited states of neutral magnesium (Weiss 1967, Robb 1974, Froese-Fischer 1975). A particular example where correlation effects are important is in the oscillator strength (length form) for the resonant $(3s^2)^1S^e - (3s3p)^1P^o$ transition. A single-configuration HF model (Weiss 1967) gives a value of about 2.4 for the oscillator strength. More sophisticated CI calculations yield values around 1.8. Since an adequate description of the atomic structure is a necessary input for an accurate scattering calculation we have chosen to represent the magnesium ground and excited states by CI wavefunctions.

A frozen-core formalism was adopted for the present calculations. The 1s, 2s and 2p orbitals were fixed by a HF calculation (using an analytic Slater-type orbital basis set) of the magnesium $(3s^2)^1S^e$ ground state. The 3s, 3p, 3d, 4s and 4p orbitals were defined by HF calculations of the $(3snl)^1L$ states. The $\bar{3}p$, $\bar{3}d$ and $\bar{4}s$ correlating orbitals were obtained by performing a natural orbital transformation (Froese-Fischer 1977)

on a large basis CI wavefunction for the $(3s^2)^1S^e$ state. All these orbitals were Schmidt orthogonalised to each other (in the order they were mentioned) and the core. A further CI calculation was used to construct the magnesium ground and excited states. Only the five lowest singlet states ($(3s^2)^1S^e$, $(3s3p)^1P^o$, $(3s4s)^1S^e$, $(3s3d)^1D^e$ and $(3s4p)^1P^o$) were included in the coupled-channels calculation. While the omission of the triplet states can undoubtedly be criticised, it is justified in the sense that the error involved is probably no larger than that arising from the use of a limited CI expansion for the target states. Moreover, we are primarily interested in elastic scattering, or in the resonant excitation to the $(3s3p)^1P^o$ state. Since the coupling between the $(3s^2)^1S^e$ and $(3s3p)^1P^o$ states is quite strong, the omission of triplet states is not expected to have a large effect.

It can be seen from table 1 that the present CI calculations give binding energies relative to the $Mg^+ 3s$ limit which are greatly improved over HF values. There are still differences between the present binding energies and the large-basis multiconfiguration Hartree-Fock (MCHF) values of Froese-Fischer (1975). This indicates that further configurations need to be included if convergence of the two-electron CI wavefunction is to be achieved. However enlarging the single-particle basis would make the electron scattering calculation prohibitively time consuming.

Table 1. Binding energies (in au) of the lowest-lying singlet states of neutral magnesium relative to the Mg^+ series limit. The energy of the CI $(3s^2)^1S^e$ ground state was -199.6460 au.

State	HF	MCHF ^a	Present	Expt
$(3s^2)^1S^e$	-0.2427	-0.276 60	-0.274 05	-0.280 99
$(3s3p)^1P^o$	-0.0994	-0.119 49	-0.114 73	-0.121 28
$(3s4s)^1S^e$	-0.0755	-0.082 13	-0.079 57	-0.082 78
$(3s3d)^1D^e$	-0.0548	-0.071 13	-0.065 76	-0.069 56
$(3s4p)^1P^o$		-0.055 66	-0.052 16	-0.055 55

^a Froese-Fischer (1975).

Another, and perhaps more stringent, test of the quality of the wavefunction can be made by computing optical oscillator strengths for the dipole-allowed transitions. This test is directly relevant to the scattering calculation, since the oscillator strengths provide a measure of the strength of the coupling between the channels. A tabulation of the present oscillator-strength values (computed with experimental energies) is given in table 2, and compared with the accurate MCHF values of Froese-Fischer (1975) and a number of experimental values. The differences between oscillator strengths computed using the length and velocity forms of the matrix element are smaller for the MCHF calculation than for our calculation. This is to be expected, since the MCHF wavefunction includes more configurations than the present CI wavefunctions. While the comparison between length and velocity oscillator strengths provides a means of testing the convergence of the wavefunctions, it is the length values that are relevant for the scattering calculations. The length value for the resonant transition differs from the MCHF f_l value by 2%.

The electron scattering calculations were done using the approach of McCarthy and Stelbovics (1983) as adapted for the use of large-dimension CI wavefunctions by

Table 2. Oscillator strengths for transitions between the low-lying singlet states of magnesium. The results using the length and velocity gauges are denoted f_l and f_v respectively. Experimental errors in the final digits are shown in parentheses.

Transition	Present		MCHF ^a		Experiment
	f_l	f_v	f_l	f_v	
$(3s^2)^1S^e - (3s3p)^1P^o$	1.728	1.600	1.757	1.736	1.83 (8) ^b , 1.83 (18) ^c 1.75 (7) ^d , 1.80 (5) ^e 1.86 (3) ^f , 1.66 (16) ^g
$(3s^2)^1S^e - (3s4p)^1P^o$	0.137	0.094	0.117	0.114	0.19 (2) ^b , 0.1022 (2) ^c 0.18 (4) ^f , 0.109 (8) ^h
$(3s3p)^1P^o - (3s4s)^1S^e$	0.184	0.145	0.155	0.155	
$(3s3p)^1P^o - (3s3d)^1D^e$	0.226	0.164	0.206	0.212	0.34 (2) ⁱ
$(3s4s)^1S^e - (3s4p)^1P^o$	0.882	1.254	1.236	1.240	
$(3s3d)^1D^e - (3s4p)^1P^o$	0.236	0.025	0.137	0.140	

^a Froese-Fischer (1975).

^b Liljeby *et al* (1980).

^c Kelly and Mathur (1980).

^d Lundin *et al* (1973).

^e Smith and Gallagher (1966).

^f Smith and Liszt (1971).

^g Andersen *et al* (1970).

^h Mitchell (1975).

ⁱ Schaefer (1971).

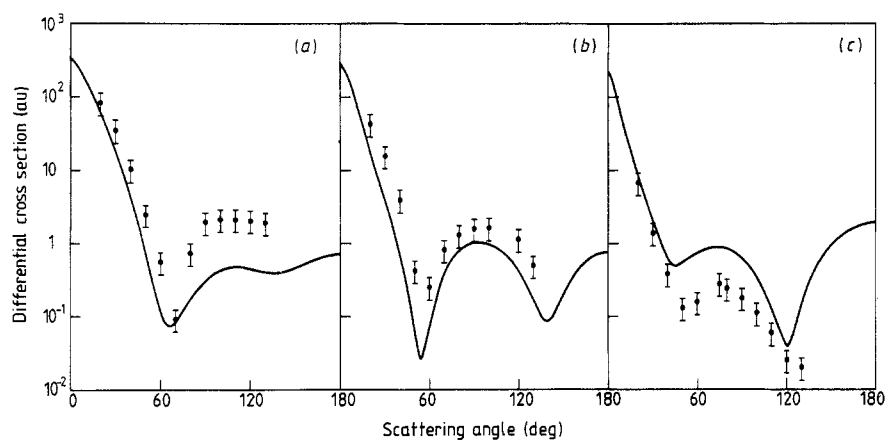
Mitroy *et al* (1987) and Bray *et al* (1988). Magnesium is represented by two valence electrons and a closed-shell core which cannot be excited but contributes direct and exchange potentials. The energy differences used in this calculation were derived from experimental energy level data. The CC equations in momentum space are a set of coupled Lippmann-Schwinger equations which are solved by discretising the continuum integral using a Gaussian quadrature rule. For the calculations reported here, the full integral equations were solved for total orbital angular momentum quantum numbers J ranging from 1 to 24. The exchange interaction was included in the kernel for $J = 0-16$. The unitarised Born approximation was used from $J = 25$ to 80 where the first Born approximation is valid. Beyond this point the first Born approximation was used to close the partial wave sum.

3. Differential and total cross sections

The differential and total cross sections for elastic scattering, calculated by the present theory, are given in table 3 for incident energies of 10, 20, 40 and 100 eV. They are compared with the experimental data of Williams and Trajmar (1978) in figure 1. The calculation compares fairly well with the experiments for small-angle elastic scattering at 10, 20 and 40 eV but for $\theta > 40^\circ$ the discrepancies are much larger. The present cross sections are substantially smaller than experiment at 10 and 20 eV, but exceed experiment at 40 eV. However, despite the differences in the absolute magnitude, the respective shapes of the experimental and theoretical cross sections are quite similar. In figure 2 we compare elastic scattering differential cross sections of neon (static exchange), sodium (four-state CC) and magnesium (five-state CC) at 100 eV. The cross sections for sodium and magnesium are much larger at smaller angles because the

Table 3. Differential and total cross sections (in a_0^2) calculated for elastic scattering from the magnesium ground state. Exponential notation is used for the power of 10.

θ (deg)	Differential cross section			
	10 eV	20 eV	40 eV	100 eV
0	3.366+2	2.838+2	2.224+2	1.611+2
5	2.732+2	2.012+2	1.280+2	6.489+1
10	1.716+2	9.142+1	4.246+1	2.521+1
20	6.173+1	1.818+1	8.849+0	6.549+0
30	1.825+1	3.693+0	2.108+0	2.211+0
40	4.322+0	7.305-1	6.107-1	1.231+0
50	7.691-1	5.507-2	5.710-1	7.608-1
60	1.176-1	7.687-2	7.735-1	5.337-1
70	8.290-2	4.150-1	9.123-1	3.673-1
80	1.761-1	7.934-1	8.599-1	2.026-1
90	3.181-1	1.004+0	6.390-1	8.545-1
100	4.452-1	9.764-1	3.580-1	2.250-2
110	4.968-1	7.465-1	1.264-1	3.716-2
120	4.693-1	4.285-1	4.005-2	1.485-1
130	4.175-1	1.714-1	1.598-1	3.393-1
140	4.060-1	8.569-2	4.842-1	6.008-1
150	4.678-1	1.996-1	9.435-1	8.920-1
160	5.835-1	4.430-1	1.421+0	1.145+0
170	6.935-1	6.801-1	1.784+0	1.323+0
180	7.341-1	7.778-1	1.918+0	1.410+0
Total	7.912+1	3.773+1	2.369+1	1.570+1

**Figure 1.** Differential cross sections for electron elastic scattering on magnesium at (a) 10 eV, (b) 20 eV and (c) 40 eV. Full circles denote the experimental data of Williams and Trajmar (1978). The full curve is the present CCs calculation.

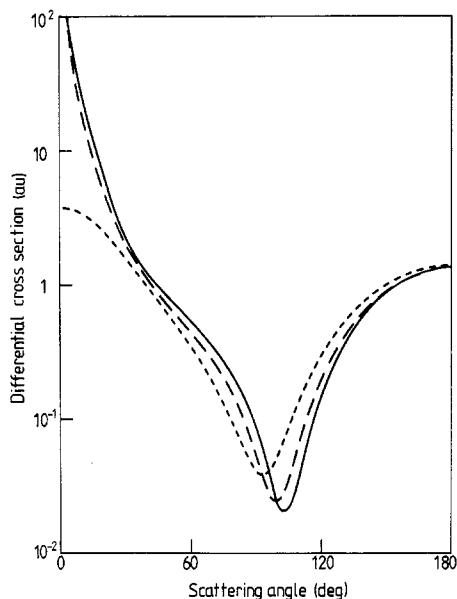


Figure 2. 100 eV elastic electron scattering from neon, sodium and magnesium. The short-dashed broken curve is the neon (static-exchange) cross section, the long-dashed broken curve is the sodium (four-state CC) cross section and the full curve is the present magnesium (five-state CC) cross section.

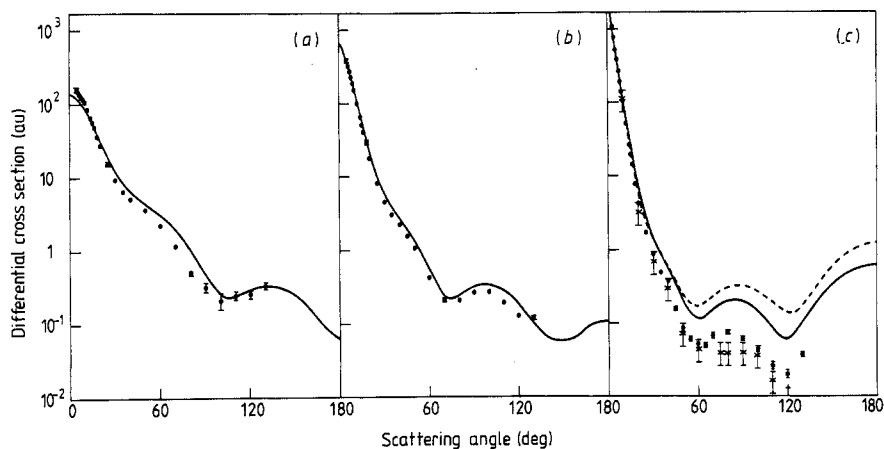
strong polarisation potential for both these atoms dominates scattering at large distances. The backward angle cross sections are similar for all these atoms, with small differences varying smoothly from neon to magnesium. This diagram demonstrates that both elastic and inelastic interactions of the scattering electron with the valence electrons have only a small influence on large-angle elastic scattering at high energies.

The differential cross sections for the resonant transition are given in table 4 and compared with the experimental data in figure 3. Agreement between theory and experiment is good at 10 and 20 eV. However, at 40 eV the cross section overestimates the magnitude of the experiment by a factor of three for $\theta > 40^\circ$ although it does correctly predict the positions of both the minima. This is reminiscent of the situation for sodium where theory greatly exceeds experiment at the highest energies. Figure 4 compares the differential cross sections for the resonant excitation of magnesium (five-state CC) and sodium (four-state CC) at 100 eV. The general shapes of the angular distributions are qualitatively similar even at backward angles, indicating that the two transitions must share the same basic reaction mechanism.

The total cross section for excitation of the resonant state of magnesium is shown in table 5 for several different calculations and compared with the emission cross section of Leep and Gallagher (1976). The present calculation is represented by CCs for the full coupled-channels value, UBA5 for the five-state unitarised Born approximation and FBA for the first Born approximation. The FBA calculation of Robb (1974) used different CI wavefunctions. The two-state close-coupling calculation of Fabrikant (1980) used dipole potential matrix elements multiplied by a constant to produce the correct optical oscillator strength and core exchange was omitted. Since the experiment of Leep and Gallagher (1976) was an emission cross section it is necessary to allow for cascades from the $(3s4s)^1S^\circ$, $(3s3d)^1D^\circ$ and $(3s4p)^1P^\circ$ levels. Since the $(3s4p)^1P^\circ$

Table 4. Differential and total cross sections (in a_0^2) calculated for the resonance $(3s^2)^1S^e - (3s3p)^1P^o$ transition in magnesium.

θ (deg)	Differential cross section			
	10 eV	20 eV	40 eV	100 eV
0	1.374+2	6.493+2	1.827+3	5.606+3
5	1.204+2	3.885+2	4.654+2	2.363+2
10	8.495+1	1.492+2	9.742+1	2.442+1
20	3.133+1	2.356+1	7.177+0	7.303-1
30	1.188+1	5.819+0	1.442+0	1.855-1
40	6.298+0	2.708+0	5.622-1	7.098-2
50	4.375+0	1.370+0	1.953-1	3.868-2
60	3.082+0	5.515-1	1.154-1	3.169-2
70	1.925+0	2.468-1	1.573-1	2.673-2
80	1.026+0	2.455-1	2.004-1	1.813-2
90	4.843-1	3.203-1	1.973-1	7.899-3
100	2.624-1	3.401-1	1.465-1	4.987-4
110	2.421-1	2.845-1	8.510-2	5.720-3
120	2.984-1	1.915-1	6.067-2	3.194-2
130	3.400-1	1.082-1	9.969-2	8.150-2
140	3.244-1	6.337-2	2.017-1	1.516-1
150	2.556-1	5.935-2	3.396-1	2.311-1
160	1.654-1	7.799-2	4.746-1	3.017-1
170	9.178-2	9.905-2	5.711-1	3.502-1
180	6.392-2	1.079-1	6.050-1	3.750-1
Total	5.301+1	5.843+1	4.860+1	2.884+1

**Figure 3.** Differential cross sections for electron scattering to the $(3s3p)^1P^o$ (first excited) state of magnesium at (a) 10 eV, (b) 20 eV and (c) 40 eV. Full circles denote the experimental data of Brunger *et al* (1988a). The full curve is the present calculation. At 40 eV the experimental data of Williams and Trajmar (1978) (crosses) and the distorted-wave Born calculation of Meneses *et al* (1987) (dotted curve) have been included for comparison.

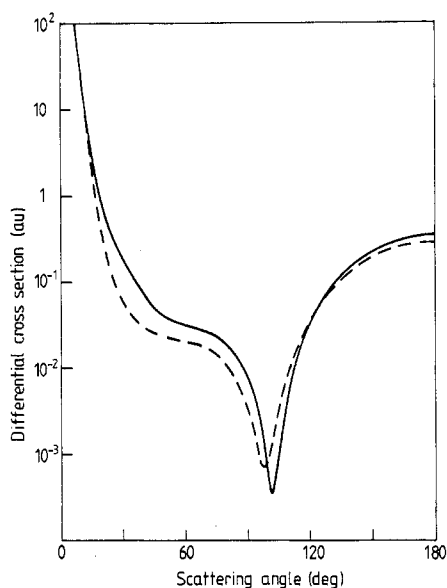


Figure 4. 100 eV electron scattering to the resonant $(3s3p)^1P^o$ state of magnesium (full curve) and the resonant $3p$ state of sodium (broken curve).

Table 5. The total cross section (in πa_0^2) for electron excitation of the resonant $(3s3p)^1P^o$ state of magnesium. CC5 is the present five-state coupled-channels calculation. UBA5 is the unitarised Born approximation to CC5 and FBA is the corresponding first Born approximation. The experimental data of Leep and Gallagher (1976) include cascade contributions. These are omitted from the theory except where indicated.

	10 eV	20 eV	40 eV	100 eV
CC5	16.9	18.6	15.5	9.5
UBA5	15.6	18.9	15.8	9.5
FBA	32.6	26.8	18.7	10.2
Robb (1974) (FBA)	42.0	—	21.8	11.6
Fabrikant (1980) (CC)	19.7	24.3	—	—
CC5 (with 4s, 4p 3d cascades)	20.2	21.3	17.4	10.4
Leep and Gallagher (1976)	16.0 (2)	17.3 (2)	15.7 (2)	10.6 (3)

level can also decay directly to the ground state the effective emission cross section is given by

$$\sigma_{\text{em}} = \sigma_{3p} + \sigma_{3d} + \sigma_{4s} + 0.137\sigma_{4p}.$$

Total cross sections for these higher levels are given in tables 6, 7 and 8. It should be noted that the MCHF f -values were used to evaluate the branching ratio for the $(3s4p)^1P^o$ level.

It is clear that the present calculations agree with total cross sections better than any of the other calculations. Although the CC5 calculation appears to agree quite well with experiment, this agreement is only coincidental since the cascade contribution

Table 6. Differential and total cross sections (in a_0^2) calculated for the $(3s^2)^1S^e-(3s4s)^1S^e$ transition in magnesium.

θ (deg)	Differential cross section			
	10 eV	20 eV	40 eV	100 eV
0	2.961+0	1.341+1	2.443+1	2.375+1
5	2.576+0	9.420+0	1.137+1	5.992+0
10	1.750+0	4.350+0	3.388+0	1.141+0
20	5.615-1	8.156-1	3.239-1	1.024-1
30	2.652-1	3.205-1	1.716-1	6.670-2
40	2.650-1	2.433-1	8.330-2	3.794-2
50	3.153-1	1.358-1	4.358-2	2.902-2
60	3.103-1	3.654-2	6.252-2	2.142-2
70	2.441-1	2.610-2	8.656-2	1.477-3
80	1.809-1	8.428-2	8.893-2	8.065-3
90	1.706-1	1.433-1	6.938-2	3.398-3
100	2.032-1	1.570-1	3.998-2	1.156-2
110	2.322-1	1.224-1	1.458-2	2.131-3
120	2.296-1	6.603-2	6.097-3	7.371-3
130	2.158-1	2.007-2	2.307-2	1.677-2
140	2.391-1	5.023-3	6.648-2	3.047-2
150	3.308-1	2.275-2	1.287-1	4.710-2
160	4.723-1	5.938-2	1.937-1	6.199-2
170	6.022-1	9.361-2	2.427-1	7.257-2
180	6.543-1	1.076-1	2.608-1	7.970-2
Total	3.630+0	2.596+0	2.039+0	8.025-1

(10–15%) leads to an effective emission cross section exceeding experiment at low energies although the agreement is good at 100 eV. One of the more notable aspects of table 5 is the excellent agreement between the UBAS and CCS calculations. The conceptually simple UBAS does amazingly well at reproducing the CCS calculation. This is somewhat fortuitous since an examination of the partial cross sections reveals that the UBAS cross section underestimates the CCS calculation for small J (e.g. $J \leq 3$) and overestimates the CCS calculation at higher J values. A similar phenomenon has also been noted for the electron impact excitation of the resonance transition in Ca^+ (Mitroy *et al* 1988).

The size of the cascade correction to the $(3s3p)^1P^o$ emission does have implications for the differential measurements of Brunger *et al* (1988a). These measurements were put on an absolute scale by integrating the differential cross section and normalising to the emission cross section of Leep and Gallagher (1976). Since the emission cross section includes cascade contributions, estimated at 10–15% corrections according to the present calculation, it is possible that the differential measurements of Brunger *et al* (1988a) systematically overestimate the actual differential cross section by 10–15%. Even if the present calculations overestimate the cascade contribution, this effect is of experimental significance since Brunger *et al* (1988b) quote absolute errors of less than $\pm 6\%$ at small angles.

The present calculation also produces total and differential cross sections for transitions to the $(3s3d)^1D^e$, $(3s4s)^1S^e$ and $(3s4p)^1P^o$ states. They are given in tables 6, 7 and 8. The cross sections for these states are not likely to be as accurate as those for elastic scattering and the resonant transition since the omission of the higher neighbouring levels from the CC expansion will have more of an influence.

Table 7. Differential and total cross sections (in a_0^2) calculated for the $(3s^2)^1S^e-(3s3d)^1D^e$ transition in magnesium.

$\theta(\text{deg})$	Differential cross section			
	10 eV	20 eV	40 eV	100 eV
0	8.361+1	2.078+1	2.814+1	3.331+1
5	7.904+0	1.689+1	1.760+1	1.467+1
10	6.706+0	1.059+1	9.236+0	5.314+0
20	3.650+0	3.381+1	2.043+0	3.721-1
30	1.495+0	9.974-1	3.580-1	8.509-2
40	5.187-1	3.471-1	1.152-1	4.368-2
50	3.153-1	2.200-1	7.553-2	2.539-2
60	2.005-1	1.776-1	5.399-2	1.349-2
70	2.498-1	1.235-1	3.432-2	7.750-3
80	2.500-1	7.712-2	2.439-2	4.945-3
90	1.882-1	5.725-2	2.388-2	3.506-3
100	1.194-1	5.724-2	2.625-2	2.774-3
110	1.001-1	6.003-2	2.558-2	2.622-3
120	1.419-1	5.466-2	2.267-2	4.707-3
130	2.104-1	4.126-2	2.339-2	1.020-2
140	2.552-1	2.674-2	3.230-2	2.005-2
150	2.456-1	1.713-2	4.824-2	3.175-2
160	6.022-1	9.361-2	2.427-1	4.375-2
170	1.277-1	1.385-2	7.977-2	5.364-2
180	1.009-1	1.430-2	8.451-2	5.520-2
Total	6.030+0	5.322+0	3.676+0	1.838+0

4. Stokes parameters

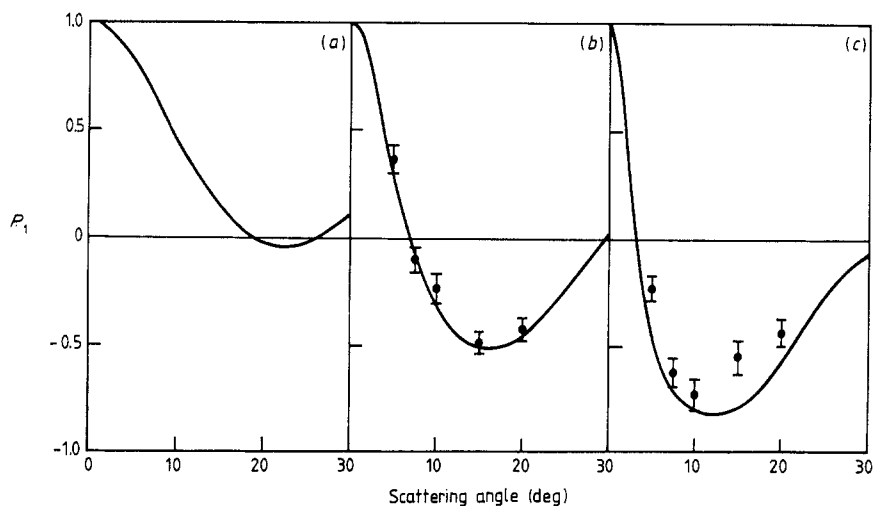
Stokes parameters for the resonant first excited state have been measured at 20 and 40 eV for an angular range $\leq 20^\circ$ by Brunger *et al* (1988b). They are compared to the experiment in figures 5, 6 and 7. There is good agreement between the theoretical and experimental measurements over the entire (although limited) angular range. It is fashionable to consider m -dependent ratios such as Stokes parameters to be a better test of a scattering theory than absolute cross sections. However, it is a moot point whether Stokes parameters taken over a restricted angular range provide a more stringent test of reaction theory than differential cross sections taken over a wider angular range. Nevertheless, additional measurements of the Stokes parameters for magnesium over a more extensive angular range would provide additional information in testing the adequacy of our present reaction theory.

5. Conclusions

We have reported results of five-state close-coupling calculations for magnesium at 10, 20, 40 and 100 eV. The qualitative agreement between theory and experiment is quite satisfactory at all energies; however the absolute magnitude of the elastic cross section is quite different from experiment. Agreement is better for the resonant transition, except for large-angle scattering at 40 eV where the theory exceeds experiment by a factor of three. There is no indication of serious departures from experiment

Table 8. Differential and total cross sections (in a_0^2) calculated for the $(3s^e)^1S^2-(3s4p)^1P^o$ transition in magnesium.

$\theta(\text{deg})$	Differential cross section			
	10 eV	20 eV	40 eV	100 eV
0	3.437+0	1.641+1	4.301+1	1.566+2
5	3.369+0	1.492+1	2.386+1	2.038+1
10	3.146+0	1.100+1	9.865+0	4.391+0
20	2.257+0	3.584+0	1.482+0	2.016-1
30	1.315+0	1.045+0	3.260-1	4.558-2
40	8.041-1	5.434-1	1.580-1	1.366-2
50	6.169-1	3.761-1	6.491-2	6.193-3
60	5.279-1	2.032-1	2.088-2	4.412-3
70	4.486-1	7.144-2	2.207-2	4.678-3
80	3.788-1	2.394-2	3.749-2	4.746-3
90	3.133-1	3.974-2	4.681-2	2.751-3
100	2.299-1	7.345-2	4.231-2	6.628-4
110	1.375-1	9.115-2	2.910-2	1.969-4
120	9.008-2	8.226-2	1.874-2	3.156-3
130	1.032-1	5.466-2	2.170-2	1.177-2
140	2.400-1	2.548-2	4.408-2	2.525-2
150	3.356-1	8.738-3	8.318-2	4.138-2
160	3.574-1	7.622-3	1.284-1	5.881-2
170	3.311-1	1.463-2	1.646-1	7.220-2
180	3.098-1	1.856-2	1.783-1	7.510-2
Total	6.166+0	5.645+0	3.944+0	2.275+0

**Figure 5.** The Stokes parameter P_1 for electron scattering to the $(3s3p)^1P^o$ (first excited) state of magnesium at (a) 10 eV, (b) 20 eV and (c) 40 eV. Black circles denote the experimental data of Brunger *et al* (1988b). The full curve is the present calculation.

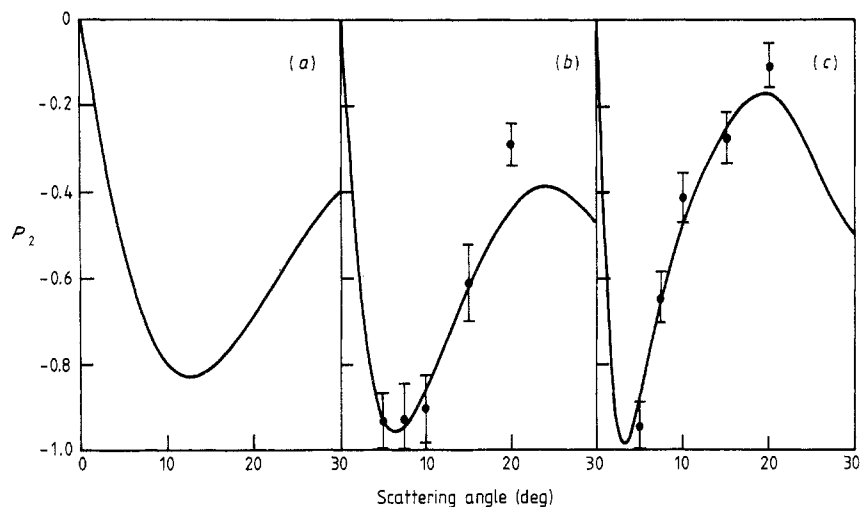


Figure 6. The Stokes parameter P_2 . For details see figure 5.

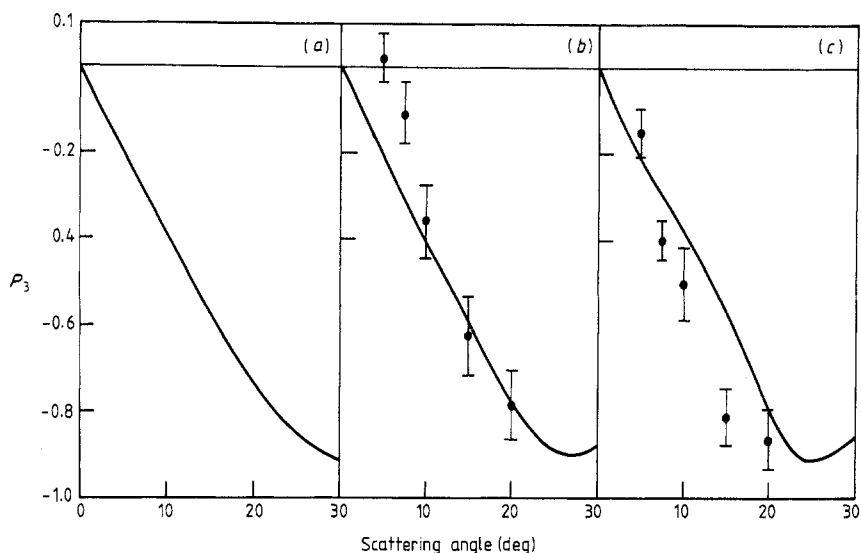


Figure 7. The Stokes parameter P_3 . For details see figure 5.

for Stokes parameters in the resonant excitation of magnesium in the restricted angular range for which data are available. The possible sources of error in the present calculation are an inadequate description of the target bound states, the omission of the target continuum and high-lying discrete states, and finally the omission of the low-lying triplet state.

The first source of error has been partially eliminated at least by using CI wavefunctions. The omission of the ionisation continuum is likely to be quite important at low energies, the total ionisation cross section reaches a maximum of $8.8\pi a_0^2$ at 12 eV (Kartensen and Schneider 1975). The omission of higher-lying states is more likely to have an effect on the $(3s3d)^1D^e$, $(3s4s)^1S^e$ and $(3s4p)^1P^o$ excitations than on the resonant

excitation, although excitations to these states will contribute to the emission cross section. We can only speculate on the possible effect of excitations to the $(3s3p)^3P$ and other triplet levels. Cross section data of Williams and Trajmar would indicate that the omission of these levels would have only a small effect at 10 and 20 eV and a negligible effect at higher energies.

Magnesium provides another target to help in the detailed understanding of electron scattering from atoms using the coupled-channels optical model. A fair description is obtained for hydrogen cross sections and for angular correlation parameters up to 60° , using optical potentials to represent excitations out of the explicitly coupled channel space (Lower *et al* 1987). For helium it is necessary to use optical potentials to obtain good total cross sections for the lowest five channels at lower energies (McCarthy *et al* 1988). For sodium it is unnecessary to use optical potentials to obtain total cross sections which agree reasonably with experiment at energies greater than 54 eV, but the differential cross sections compare very poorly with experiment for $\theta > 20^\circ$ (Mitroy *et al* 1987). At present it is a matter of contention whether the discrepancies between theory and experiment at higher energies and large angles are due to theoretical or experimental inadequacies. Differential cross sections for magnesium are reminiscent of those for sodium. The comparison of theory and experiment at 40 eV provides a strong indication that the theory at higher energies will overestimate the experiment considerably at larger angles. Since the program used for the present calculation was used for the prior sodium calculations, and the experimental apparatus used for the recent magnesium experiment (Brunger *et al* 1988a) was the same as that used for the recent sodium experiment (Teubner *et al* 1986), it is clear that independent calculations and experiments will be valuable in resolving the current discrepancies.

Total cross sections for the first excited state of magnesium in the present calculation compare only fairly well with experiment. The experience with helium at lower energies suggests that the addition of optical potentials will cause a decrease in the total cross section for resonant excitation.

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