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The Elastic Scattering of 20 eV Electrons from Magnesium

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Abstract

A modulated crossed-beam technique has been used to measure the differential cross section for elastic scattering of electrons from the 3^1S state in magnesium at an impact electron energy of 20 eV. The cross section was measured over a range of scattering angles from 15° to 130°. Our results agree with the previous experimental cross sections of Williams and Trajmar within the combined uncertainties, however, the present data reduce the uncertainty by about an order of magnitude, thereby allowing a meaningful comparison to be made with the predictions of the various theories. At this time no theory accurately predicts the behaviour of the elastic differential cross section over the whole angular range. A complex phase-shift analysis is applied to the present data to derive the 20 eV integral elastic cross section. This integral cross section is also compared with the results of previous experiment and theory.

1. Introduction

The recent extension of the convergent close-coupling technique to 'two electron' atoms by Bray *et al.* (1994) has opened up the possibility of applying this technique to the electron–magnesium scattering problem. Although Williams and Trajmar (1978) have reported an extensive set of differential cross sections for electron scattering from magnesium, the large uncertainties in their data do not make them a very discriminating test for the validity of any or all of the 2-state close-coupling (CC) calculation of Fabrikant (1980), the optical potential calculation of Khare *et al.* (1983), the energy-dependent real model potential calculation of Keleman *et al.* (1989), the 5-state CC calculation of Mitroy and McCarthy (1989), the 6-state CC optical model calculation of McCarthy *et al.* (1989), the 10-state CC result of Zhou (1994) and, in particular, of a sophisticated calculation of the type performed by Bray *et al.* (1994). The present 20 eV elastic differential cross section data, with uncertainties that are reduced by an order of magnitude compared with those reported by Williams and Trajmar (1978), are presented to provide the same stringent test for the theory in the elastic channel, as that provided by the differential cross sections of Brunger *et al.* (1988), for the 3^1P state, and the differential and integral cross sections of Houghton *et al.* (1994), for the 3^3P state.

By their very nature, integral cross sections, where angular information is integrated out, provide a less sensitive test of the validity of a calculation than the

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corresponding differential cross sections. Nonetheless, they still provide a measure of the quality of a given calculation, and in many applications, such as laser and discharge modelling, are actually the important quantity in the modelling process. Consequently, we have applied the complex phase-shift analysis of Allen *et al.* (1987) to the present differential cross section in order to provide an unambiguous method of extrapolating the data to 0° and 180°, before integration, to generate our 20 eV integral elastic cross section.

The experimental procedure is briefly described in Section 2, as is the phase-shift analysis, whilst our results are presented and discussed in Section 3.

2. Experimental Technique and Assignment of Absolute Values

A modulated crossed-beam apparatus, as described in Brunger *et al.* (1988), was used to measure the present magnesium elastic differential cross sections. These measurements involve the observation of the angular distribution of elastically scattered electrons. At a particular angle, θ, the energy of the scattered signal was analysed by a cylindrical mirror electron spectrometer which viewed the interaction region defined by the intersection of the neutral magnesium beam and the electron beam. The selected elastic signal was then detected by the channel electron multiplier (CEM) and the pulses from the CEM amplified and counted in either of two gated scalers. The gates of the scalers were activated by a reference signal produced by the modulation of the magnesium beam. One scaler was enabled when the beam was in the interaction region, thus counting the scattered signal from both the beam and the background, $N_{\rm a}$. The other scaler was enabled when the beam was off, and counted $N_{\rm b}$, the background signal. After a preset time, the difference was proportional to the number of electrons elastically scattered from the neutral beam, at a particular angle θ. The relative elastic angular distribution, $N_{\rm el}(\theta)$, was obtained by repeating this procedure at each scattering angle.

The relative elastic angular distribution was placed on an absolute scale using a method similar to that described in Houghton *et al.* (1994). The absolute differential cross section, $\sigma_{\rm el}(\theta)$, is related to the relative angular distribution by

$$\sigma_{\rm el}(\theta) = C N_{\rm el}(\theta)\,, \tag{1}$$

and at the normalising angle, θ_0, is related to the differential cross section for the excitation of the 3^1P state in magnesium by

$$\sigma_{\rm el}(\theta_0) = R_{\theta_0}\, \sigma_{3^1{\rm P}}(\theta_0)\,, \tag{2}$$

where $\sigma_{3^1{\rm P}}(\theta_0)$ is the known differential cross at θ_0 as measured by Brunger *et al.* (1988) and R_{θ_0} is the experimental ratio of the elastic signal to the inelastic 3^1P signal at the normalising angle θ_0. The normalising constant, C, which in a carefully conducted experiment is independent of scattering angle, can then be calculated from equations (1) and (2). This constant C was then used to convert the measured relative angular distribution into an absolute elastic differential cross section.

Considerable care has been exercised to identify and remove potential sources of systematic error in the present measurements. These precautions are discussed in detail elsewhere (Brunger *et al.* 1988; Houghton *et al.* 1994) and so are not repeated here.

To derive the integral elastic cross section from the differential cross section data reported here, the present data need to be extrapolated to scattering angles of 0° and 180°. The phase-shift analysis technique of Allen *et al.* (1987) was used to provide an unambiguous method of extrapolating the data. This phase-shift analysis was based on the method of Allen (1986) generalised to the complex case. However, as a detailed description of the complex phase-shift technique can be found in Allen *et al.* (1987), we do not repeat the details here.

3. Results and Discussion

The differential cross sections for the elastic scattering of electrons from magnesium at 20 eV are given in Table 1. Absolute values were assigned using the prescription described in Section 2. The errors shown were obtained by adding the error in the normalisation constant in quadrature with the statistical error in the elastic angular distribution at each scattering angle.

Table 1. Differential cross sections for elastic scattering from the 3^1S state in magnesium of electrons of energy 20 eV

Angle θ (deg)	Differential cross sections ($a_0^2\,\mathrm{sr}^{-1}$)
15	7·97 E+01 ± 4·33 E+00
20	4·90 E+01 ± 2·58 E+00
25	2·29 E+01 ± 1·19 E+00
30	1·07 E+01 ± 5·59 E−01
35	4·46 E+00 ± 2·40 E−01
40	1·68 E+00 ± 1·09 E−01
45	9·87 E−01 ± 7·70 E−02
50	4·85 E−01 ± 5·86 E−02
52·5	2·11 E−01 ± 8·41 E−02
60	7·80 E−02 ± 2·94 E−02
62·5	1·97 E−01 ± 2·89 E−02
65	4·14 E−01 ± 3·78 E−02
70	8·73 E−01 ± 5·13 E−02
80	1·61 E+00 ± 8·52 E−02
90	1·84 E+00 ± 9·91 E−02
100	1·82 E+00 ± 9·53 E−02
110	1·31 E+00 ± 7·24 E−02
120	7·69 E−01 ± 5·62 E−02
125	5·74 E−01 ± 7·13 E−02

In Fig. 1*a* the present results are compared with the predictions of the 2-state CC calculation of Fabrikant (1980), the optical potential calculation of Khare *et al.* (1983), and with the energy-dependent real model potential calculation of Keleman *et al.* (1989). The present results are also compared with the previous experimental elastic cross sections of Williams and Trajmar (1978). Both experimental cross sections are in good agreement within the combined uncertainties. However, the present data reduce the uncertainty by almost an order of magnitude, thus allowing a more discriminating comparison between the experiment and the predictions of the theoretical calculations.

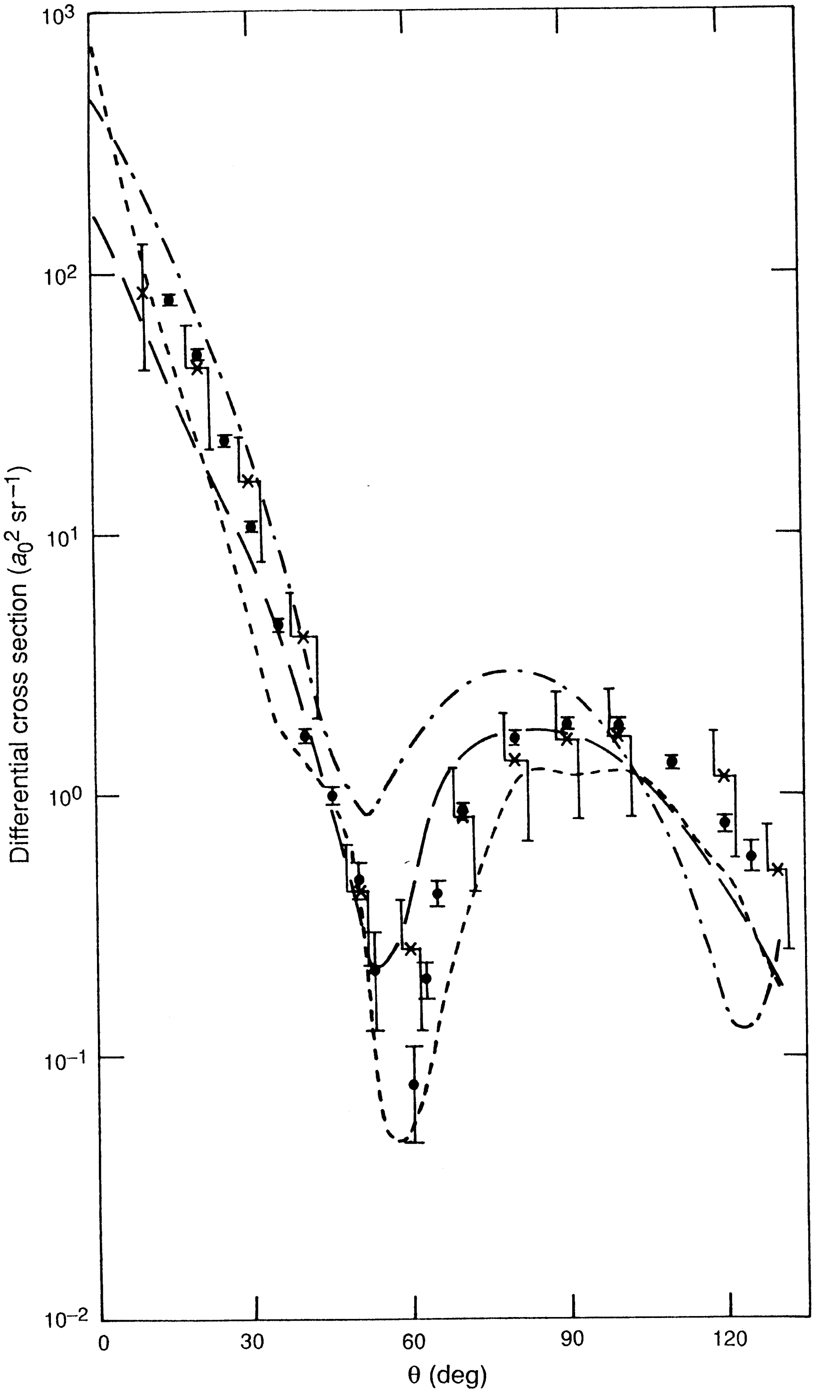

Fig. 1*a*. Absolute differential cross section for the elastic scattering of 20 eV electrons from magnesium. The present results, ●, are compared with the data of Williams and Trajmar (1978), ×, and with the predictions of the optical potential calculation of Khare *et al.* (1983), –·–·, the energy-dependent real model potential calculation of Keleman *et al.* (1989), ––, and the 2-state CC calculation of Fabrikant (1980), ---.

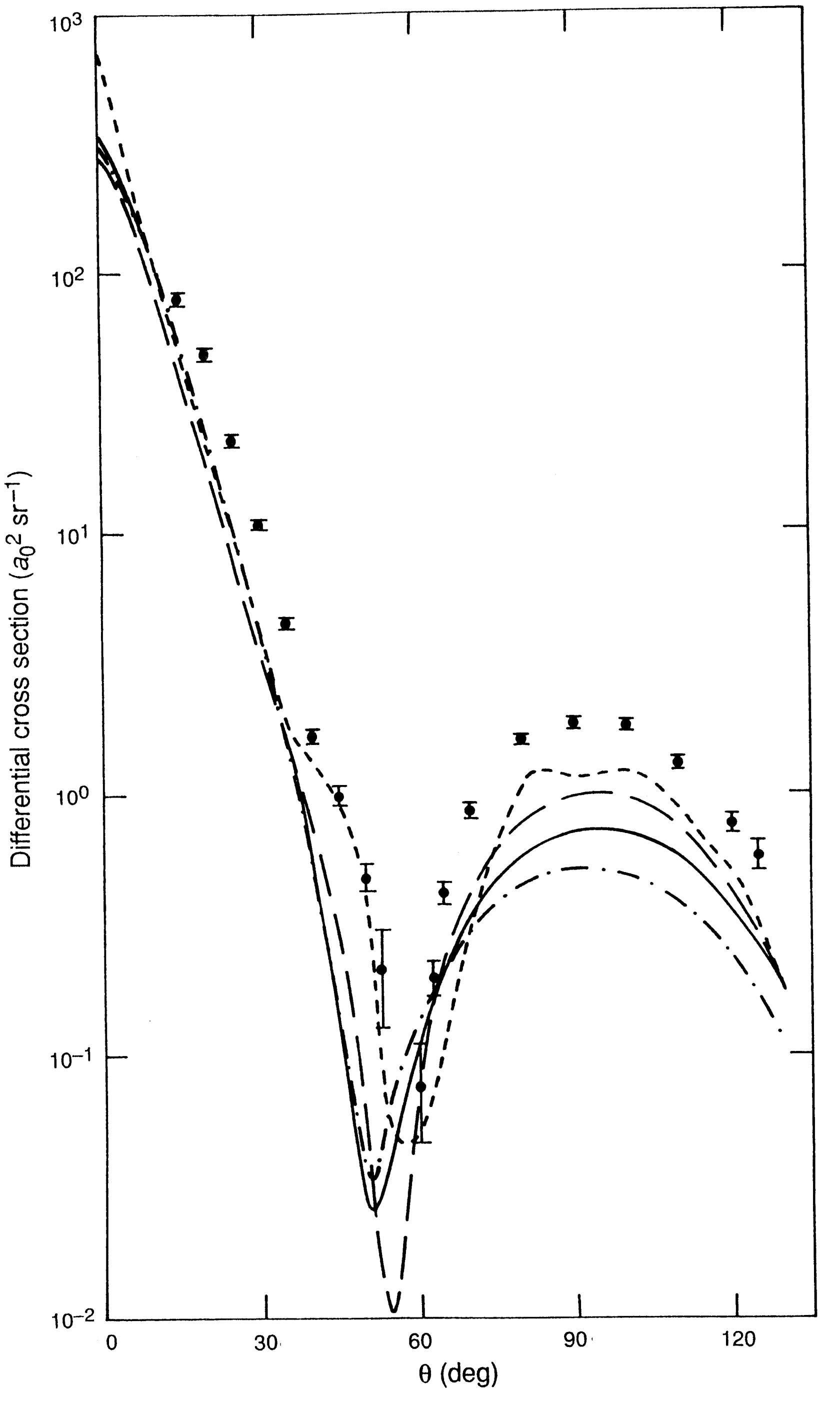

Fig. 1*b*. Absolute differential cross section for the elastic scattering of 20 eV electrons from magnesium. The present results, ●, are compared with the predictions of the 2-state CC calculation of Fabrikant (- - -), the 5-state CC calculation of Mitroy and McCarthy (1989), – –, the 6-state CC optical model calculation of McCarthy *et al.* (1989), – · – ·, and the 10-state CC calculation of Zhou (1994), —.

None of these theoretical calculations provides substantial quantitative agreement with the present results over the whole angular range. The optical potential calculation of Khare *et al.* (1983) predicts the shape of the differential cross section at forward angles ($\theta_e < 50°$), but shows substantial disagreement with the present results at middle and backward angles. This theory predicts a second minimum in the cross section at 120° which is not observed in the experimental data. In contrast, the energy-dependent potential calculation of Keleman *et al.* (1989), while providing a better description of the differential cross section at middle and backward angles than the calculation of Khare *et al.*, significantly underestimates the cross section data at forward angles.

The 2-state CC calculation of Fabrikant (1980) successfully predicts the minimum in the cross section at middle angles, and provides the most accurate description of the shape of the cross section over the whole angular range. However, this 2-state close-coupling calculation underestimates the cross section at backward angles and in the forward angular region.

In Fig. 1*b* the present data are compared with the predictions of the 2-state CC calculation of Fabrikant (1980), the 5-state CC calculation of Mitroy and McCarthy (1989), the 6-state coupled-channel optical model calculation of McCarthy *et al.* (1989), and with the 10-state CC calculation of Zhou (1994). The 2-state CC calculation is the most successful of these theoretical calculations, predicting the minimum at approximately 60° and the ledge in the differential cross section data in the angular region from 35° to 50°. Somewhat surprisingly, the more sophisticated calculations of McCarthy and co-workers provide less accurate descriptions of the shape of the cross section, and significantly underestimate the cross section at backward angles.

It is unlikely that the observed disagreement between experiment and theory, in particular the disagreement with the calculations of McCarthy and co-workers, could be due to a problem with the normalisation procedure, as the 3^1P differential cross section of Brunger *et al.* (1988) at 20 eV was found to be in very good agreement with these same calculations over the entire angular range. Bray *et al.* (1994) have recently found that to obtain good agreement between theory and experiment for electron scattering from helium, it was necessary to apply their convergent CC model. In this 62-state calculation, sophisticated models for both the continuum and exchange were necessary before the detailed agreement with experiment that they found was obtained. We believe that such a detailed calculation will also be necessary for magnesium before substantive agreement with experiment will be achieved.

The smooth curve fit from the phase-shift analysis was found to be in good agreement with the present experimental data. In the present analysis, 12 free parameters ($N = 3$) were used to fit 19 experimental data points. The initial values for the 12 free parameters a_n were obtained by fitting the real and imaginary phase shifts for $\ell = 0, 1, 2, 3$ generated by the 6-state CC calculation of McCarthy *et al.* (1989) using the parametrisation of the S-matrix. The fitted theoretical parameters a_n were then used as the starting point for the minimisation of χ^2 for the experimental data.

The applicability of the method to the present study was confirmed by the quality of the fit. The parametrisation generated phase shifts for all ℓ and it was found that the fit converged to the experimental data for $\ell = 200$. The measure of success of a least-squares fit is a value of χ^2 which on average is close to one. In the present analysis a χ^2 value of $5 \cdot 6$ was obtained, which is, on the surface, somewhat disappointing. This initial concern was tempered by the observation that the fitted curve lies within the error bars of the experimental data at almost every data point. Allen *et al.* (1987) have previously discussed the effect of non-statistical errors on the value of χ^2 obtained with a parametrisation similar to that used in the present study. They found that the value of χ^2 could be significantly reduced by allowing very small horizontal shifts in the measured elastic differential cross section, within the uncertainty in the value of the scattering angle. Full details of this procedure can be found in Allen *et al.* (1987). In the present case by simply shifting the 20° point by $-0 \cdot 2°$, the 40° point by $+0 \cdot 5°$ and the 50° point by $-0 \cdot 5°$, the value of χ^2 was decreased significantly from $5 \cdot 60$ to $1 \cdot 98$. This dramatic effect on χ^2 can be understood in view of the observation that the dynamic range of the cross section varied by a factor of about 1000 in going from 15° to 60°.

The total elastic cross section derived from the phase shift analysis is given in Table 2, where it is compared with previous experimental and theoretical cross sections reported in the literature. The present total cross section value is in reasonable agreement with the value reported by Williams and Trajmar (1978), who did not report an error in their value. However, all the theoretical cross sections tabulated in Table 2 are smaller than the total elastic cross section reported here. This behaviour is not surprising as the elastic differential cross sections predicted by these theories, particularly at forward angles, also underestimate the differential cross section measured in the present study (see Fig. 1*b*).

Table 2. Integral elastic cross section for scattering from magnesium at 20 eV

	Total elastic cross section (πa_0^2)
Present	$20 \cdot 6 \pm 2 \cdot 02$
Williams and Trajmar (1978)	18·2
Fabrikant (1980)	14·0
Mitroy and McCarthy (1989)	12·0
McCarthy *et al.* (1989)	14·9
Zhou (1994)	12·7

The large statistical uncertainty in the total cross section derived from the phase shift analysis reflects the limited angular range of the experimental differential cross section data, in particular, the absence of data points at very forward angles. In the present study, differential cross section data were not measured at angles less than 15° due to interference from the primary electron beam. The fitting procedure was therefore unable to accurately define the fit at very forward angles where the differential cross section is strongly peaked and contributes significantly to the total elastic cross section. It should be noted that Williams and Trajmar (1978) made no measurements at scattering angles less than 20°, and it is unclear how they extrapolated their differential cross section data to 0° and 180° scattering angles. This phase-shift analysis shows that this is a crucial kinematical region for the determination of the total elastic cross section.

Acknowledgments

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