

## Calculation of electron scattering cross sections for magnesium and barium

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Received 9 May 1979

**Abstract.** Differential and integral cross sections for elastic scattering and excitation of Ba and Mg atoms were calculated by solving the close-coupling equations including the ground and resonance target states. In the valence shell of an atom the configuration interaction was approximately taken into account by a simple procedure. The contribution of the highest partial waves to the cross sections was calculated either in the Bethe approximation (for excitation) or in its modification (for elastic scattering). The polarisation of the resonance lines radiation was also obtained. The energy dependence of the excitation cross section and polarisation in the region from threshold to 35 eV are presented for Ba. Comparison with experimental data shows that strict consideration of the configuration interaction is necessary. The effect of this interaction is most important in the region of the excitation cross section maximum.

### 1. Introduction

In previous theoretical works on electron scattering by alkaline earth atoms (Fabrikant 1974, 1975) elastic and excitation cross sections were calculated by the close-coupling method for low electron energies (to 8 eV). Recently the differential cross sections for electron scattering by Mg and Ba have been measured (Williams and Trajmar 1978, Jensen *et al* 1978). These results provide an opportunity to consider theoretical data more critically because the differential cross sections contain more information about scattering than the integral ones.

In the present paper the differential cross sections for electron scattering by Ba and Mg atoms calculated by a close-coupling method are given. For Ba the energy dependence of the integral cross sections and the polarisation of radiation to 35 eV is also presented. More extensive data on elastic differential cross sections by Ba are given elsewhere (Fabrikant 1979).

### 2. The choice of initial approximations

In the previous papers (Fabrikant 1974, 1975) on the electron scattering by alkaline earth atoms, close-coupling approximations with  $\{n^1S, n^1P\}$ ,  $\{n^1S, n^1P, n^3P\}$  and  $\{n^1S, n^1P, (n-1)^1D\}$  basis sets were used, where  $n$  is the principal quantum number of the target ground state. If the energy of the incident electron increases, the usual problem of taking into account additional open channels arises. Results of the calculation of scattering by alkaline (Moores and Norcross 1972) and alkaline earth

atoms show that for energies which are not too low the cross section for elastic scattering and excitation of the resonance level can be obtained with good accuracy in the  $nS$ – $nP$  approximation, and the additional channels may be ignored. This opportunity is caused by a strong coupling between the  $nS$  and  $nP$  states. This coupling is much stronger than the coupling of the  $nS$  state with any other state. It can be seen, for example, from the comparison of the cross section for excitation of Mg  $3^1P$  state with the cross section for excitation of the  $3^3P$ ,  $3^1D$ ,  $4^1S$  and  $4^1P$  states (Williams and Trajmar 1978).

Therefore, in the present paper we retain only  $n^1S$  and  $n^1P$  states in the close-coupling expansion. It was shown (Fabrikant 1975) that  $6^1P$ – $5^1D$  coupling essentially influences the cross section for excitation of the  $6^1P$  state of Ba near threshold. However, for energy  $E > 8$  eV this coupling becomes insignificant. Calculations show that if the energy increases, the main contribution to the excitation cross section is given by the partial waves with large  $L$  for which the influence of the  $6^1P$ – $5^1D$  coupling is small (see figure 3 below).

In the previous calculations it was also found that when the electron is scattered by the alkaline earth atoms, in an atom valence shell the configuration interaction is of great importance. For an accurate account of this effect one needs calculations with configuration-interaction wavefunctions (Van Blerkom 1970, Robb 1975). As a first step the following simple procedure may be proposed.

Note that mixing of  $ns^2$  and  $np^2$  configurations is most essential for the ground state of alkaline earth atoms, and the mixing of  $nsnp$  and  $np(n-1)d$  configurations is most essential for the resonance state. (For Be and Mg the last configuration is absent.) Thus, the wavefunctions of these states may be written in the form (Kim and Bagus 1972):

$$\begin{aligned}\psi_S &= a\phi(ns^2) + b\phi(np^2) \\ \psi_P &= a'\phi(nsnp) + b'\phi(np(n-1)d)\end{aligned}\quad (1)$$

where  $\phi$  is the one-electron (e.g. Hartree–Fock) wavefunction of the valence shell for the configuration given in brackets.

Now consider the corrections to the direct potentials caused by the configuration interaction. The correction to the potential  $V_{S \rightarrow S}$  is proportional to  $b^2$  and may be neglected, since  $b$  is rather small. If we are not interested in the cross section for scattering from the  $n^1P$  state, the correction to potential  $V_{P \rightarrow P}$  can also be omitted. Thus, the potential

$$V_{S \rightarrow P}(r_3) = \int \psi_S^*(r_1, r_2) V(r_1, r_2, r_3) \psi_P(r_1, r_2) dr_1 dr_2 \quad (2)$$

remains where  $V(r_1, r_2, r_3)$  is the interaction between the incident and valence electrons.

Supposing that the radial orbitals do not depend on the electron configuration we obtain from (1) and (2)

$$V_{S \rightarrow P} = c V_{S \rightarrow P}^0 \quad c = a'(a - b/\sqrt{3}) \quad (3)$$

where  $V_{S \rightarrow P}^0$  is the potential  $V_{S \rightarrow P}$  obtained with the configuration interaction ignored.

Approximation (3) for the oscillator strength of the resonance transition gives

$$f = c^2 f^0 \quad (4)$$

Therefore, the coefficient  $c$  can be obtained by fitting the value of  $f$ , following from (4), to the result of a configuration-interaction calculation. In the present work, as well as in the previous one, semi-empirical wavefunctions for the valence electron (Anderson *et al* 1967, Zilitis 1970) were used. These functions give  $f^0 = 2.12$  for Mg and  $f^0 = 2.52$  for Ba. From the analysis of the results of the configuration-interaction calculations (Weiss 1967, Friedrich and Trefftz 1969, Kim and Bagus 1972, Robb 1974) we have chosen  $f = 1.81$  and  $f = 1.65$  respectively which gives  $c = 0.925$  and  $c = 0.809$ .

This approach allows us to take into account correctly, the long-range part of the potential  $V_{1s-1p}$ . However, approximation (3) does not allow us to state the same about the short-range part of the  $V_{1s-1p}$ . Besides, the approach neglects the modification of the exchange potentials and the short-range potential  $V_{1s-1s}$  which may influence the the elastic scattering cross sections essentially.

It should be also mentioned that in the present calculations we neglect the exchange between the incident and atomic core electrons, polarisation of the atomic core and spin-orbit interaction. The last two effects are unimportant for Mg, but may be essential for Ba.

### 3. Calculations

#### 3.1. The account of the highest partial waves

The close-coupling equations were solved in the same way as in the previous works (Fabrikant 1974, 1975). If the energy increases, the essential feature of the calculations is that more partial waves should be taken into account. For this purpose we may use the Bethe approximation for the excitation cross sections. Then the amplitude for the excitation of the sublevel with magnetic quantum number  $M$  has the form

$$f_M(\theta, \phi) = f_M^{(B)}(\theta, \phi) - \left( \frac{\pi}{k_0 k_1} \right)^{1/2} \sum_{L=0}^{L_m} (2L+1)^{1/2} [(T_{01}^L - T_{01}^{L(B)}) \times (1, L-1, M, -M|L0) Y_{L-1, -M}(\theta, \phi) - (T_{02}^L - T_{02}^{L(B)}) \times (1, L+1, +M, -M|L0) Y_{L+1, -M}(\theta, \phi)] \quad M = 0, \pm 1 \quad (5)$$

where  $L_m$  is the maximum total moment  $L$  for which calculations are carried out by the close-coupling method;  $(1, L \pm 1, M, -M|L0)$  are Clebsch-Gordan coefficients;  $Y_{l, -M}$  is a normalised spherical harmonic;  $T_{01}^L, T_{02}^L$  denote the  $T$  matrix elements for a transition from the ground state to the channels with the electron angular momentum  $L-1$  and  $L+1$ ;  $T_{01}^{L(B)}, T_{02}^{L(B)}$  denote the same elements in the Bethe approximation:

$$T_{01}^{L(B)} = 2i\pi^{1/2} \beta \left( \frac{L}{2L+1} \right)^{1/2} z^{L/2-1/4} \frac{\Gamma(L)}{\Gamma(L+\frac{1}{2})} F(L, -\frac{1}{2}; L+\frac{1}{2}; z) \\ T_{02}^{L(B)} = -i\pi^{1/2} \beta \left( \frac{L+1}{2L+1} \right)^{1/2} z^{L/2+3/4} \frac{\Gamma(L+1)}{\Gamma(L+\frac{5}{2})} F(L+1, \frac{1}{2}; L+\frac{5}{2}; z) \quad (6)$$

where  $F$  is the hypergeometric function,  $\Gamma$  is the gamma function,  $z = k_1^2/k_0^2$ ;  $k_0, k_1$  are electron wavenumbers;

$$\beta = \left( \frac{2}{3} \right)^{1/2} c \int u_0(r) r u_1(r) dr$$

where  $u_0, u_1$  are the radial atomic orbitals for the ground and excited states and  $c$  is defined by (4).

The excitation amplitude in the Bethe approximation has the form:

$$f_0^{(B)} = -\frac{2i\beta}{q^2}(k_0 - k_1 \cos \theta) \quad f_{\pm 1}^{(B)} = -\frac{2^{1/2}i\beta}{q^2}k_1 \sin \theta e^{\mp i\phi}$$

$$q^2 = k_0^2 + k_1^2 - 2k_0k_1 \cos \theta. \quad (7)$$

To account for the highest partial waves when calculating elastic cross sections one may use the following expression for  $T_{00}^L$ :

$$T_{00}^L = -2iK_{00}^{L(M)} + 2(K_{01}^{L(B)})^2 \quad (8)$$

where  $K_{00}^{L(M)}$  is the  $K$  matrix element calculated by the formula of the modified effective range theory (O'Malley *et al* 1961) for scattering by the polarisation potential  $\beta^2/(\epsilon r^4)$  ( $\epsilon$  is the excitation energy),  $K_{01}^{L(B)} = -T_{01}^{L(B)}/2i$ . Approximation (8) is less exact than the unitarised Born approximation but it is quite sufficient for our purpose.

Using the asymptotic expression for  $K_{01}^{L(B)}$  at large  $L$

$$K_{01}^{L(B)} \sim -\beta \left( \frac{\pi}{2L+1} \right)^{1/2} z^{L/2-1/4} (1-z)^{1/2}$$

one can give the highest wave addition to the elastic scattering amplitude in the form

$$\Delta f = \frac{\pi\beta^2}{k_0} \sum_{L=L_m+1}^{\infty} \left( iz^{L-1/2}(1-z) + \frac{2k_0^2}{\epsilon(2L-1)(2L+3)} \right) P_L(\cos \theta)$$

$$= -\frac{\pi\beta^2}{k_0} \sum_{L=0}^{L_m} \left( iz^{L-1/2}(1-z) + \frac{2k_0^2}{\epsilon(2L-1)(2L+3)} \right) P_L(\cos \theta)$$

$$+ \pi\beta^2 \left( \frac{i}{k_1} \frac{1-z}{(1+z^2-2z \cos \theta)^{1/2}} - \frac{k_0}{\epsilon} \sin \frac{1}{2}\theta \right). \quad (9)$$

In our calculations  $L_m$  varied with the change of energy from 8 to 16 to provide good convergence for the scattering amplitudes.

### 3.2. Polarisation of radiation

According to the theory of Percival and Seaton (1958) the polarisation of atomic radiation excited by electron impact for an isotope mixture with different nuclear spins can be obtained from the formula

$$P = \frac{\sum_i (3K_z^{(i)} - K^{(i)})c^{(i)}}{\sum_i (K_z^{(i)} + K^{(i)})c^{(i)}} \quad (10)$$

where  $K_z^{(i)}$  is the rate coefficient for emission of photons characterised by the electric dipole lying in the  $z$  direction,  $K^{(i)}$  is the rate coefficient for emission of all the photons,  $c^{(i)}$  is the isotope concentration. Summation is carried out over isotopes with different nuclear spins.

Let  $I = 0$  for all Mg isotopes since according to the conclusion of Leep and Gallgher (1976) the hyperfine structure of the  $^{25}\text{Mg } 3^1\text{P}$  level is thought to be much smaller than the natural level width. Then

$$P = (Q_0 - Q_1)/(Q_0 + Q_1) \quad (11)$$

where  $Q_M$ ,  $M=0, 1$  are the cross sections for the excitation of the sublevels with magnetic quantum number  $M$ .

Natural Ba contains 18% of the isotopes  $^{135}\text{Ba}$  and  $^{137}\text{Ba}$  with  $I = 3/2$ . Other stable isotopes have  $I = 0$ . The hyperfine structure of  $^{135}\text{Ba}$ ,  $^{137}\text{Ba}$   $6^1\text{P}$  is large compared with the natural level width (Lurio 1964). Therefore from the Percival and Seaton (1958) it follows that:

$$K_Z^{(1)} = \frac{Q_0}{Q_0 + 2Q_1} K \quad K_Z^{(2)} = \frac{112Q_0 + 113Q_1}{225(Q_0 + 2Q_1)} K \quad K^{(1)} = K^{(2)} = K.$$

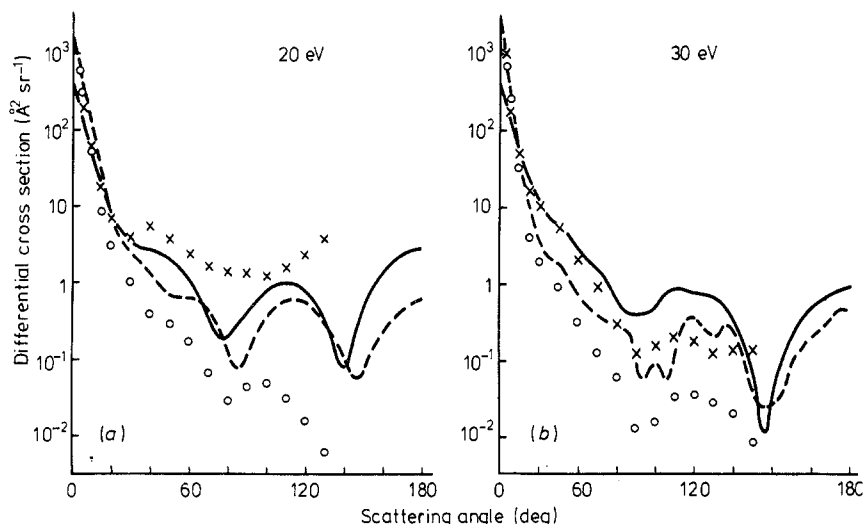
Substituting these expressions in formula (10) and noting that  $C^{(1)} = 0.82$ ,  $C^{(2)} = 0.18$  we obtain

$$P = \frac{Q_0 - Q_1}{1.104Q_0 + 1.210Q_1} \quad (12)$$

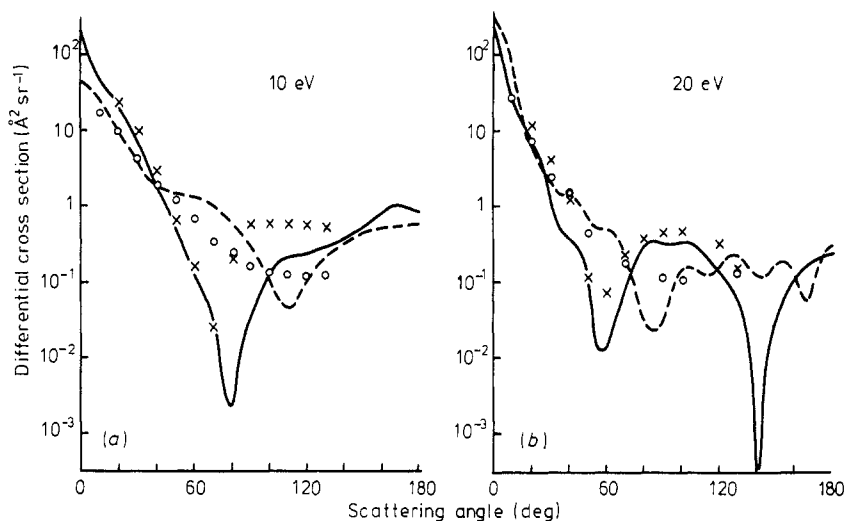
and  $Q_M$  can be obtained from amplitude (5).

#### 4. Results and discussion

The differential cross sections for the elastic scattering and excitation of Ba and Mg are presented in figures 1 and 2. The experimental points of Jensen *et al* (1978) and Williams and Trajmar (1978) are also given. The shapes of experimental and theoretical curves coincide quite well but disagreement is observed for absolute values of the cross sections in the region of large scattering angles. This disagreement is not large for Mg, because we have to take into account the limited angular resolution of the detector used in the experiment.



**Figure 1.** Differential cross sections for scattering by Ba atoms at (a) 20 and (b) 30 eV. Experimental points of Jensen *et al* (1978) are:  $\times$ , elastic;  $\circ$ , excitation. Theoretical results are: full curve, elastic scattering and broken curve, excitation.



**Figure 2.** The same as in figure 1 for Mg atoms and electron energies of (a) 10 and (b) 20 eV. Experimental points are from the work of Williams and Trajmar (1978).

However, for Ba at  $\theta > 60^\circ$  disagreement is rather large and is not within an experimental error. It would be reasonable to assume that the disagreement is caused by neglecting the core polarisation and spin-orbit interaction, which are inessential for Mg, and by inaccurate account of configuration interaction. The latter effect is also less important for Mg. Approximation (3) takes into account the long-range interaction correctly. Thus, at small scattering angles the agreement between the theory and the experiment is better.

Williams and Trajmar (1978) and Jensen *et al* (1978) obtain absolute values of the cross sections by integrating differential excitation cross sections and normalising the results obtained to the excitation functions of Leep and Gallagher (1976) and Chen and Gallagher (1976). Due to the difficulties of the experimental data extrapolation to small and large scattering angles, Williams and Trajmar and Jensen *et al* estimate the accuracy of their results to be within  $\pm 50\%$  (for the magnitude of the cross section). Note that the essential contribution to the integral cross sections is given by the region of small scattering angles, because here the differential cross section varies very rapidly and the experimental angular resolution is limited to  $2^\circ$  for Mg and  $1^\circ$  for Ba. Therefore, good agreement of the excitation cross sections at small scattering angles (see figure 1) is insufficient for the coincidence of the integral magnitude. For example, at  $E = 20$  eV the theoretical contribution from the  $0-3^\circ$  region to the integral excitation cross section is  $11.4 \pi a_0^2$  but the result of the Jensen *et al* (1978) extrapolation gives  $5.6 \pi a_0^2$ . For contribution from  $3^\circ$  to the  $15^\circ$  region values are  $33.8 \pi a_0^2$  and  $21.9 \pi a_0^2$  respectively.

The integral elastic cross sections are listed in table 1. Cross sections for scattering into the back hemisphere are also presented for the characteristic of the contribution from the  $\theta > 90^\circ$  region:

$$Q_h = 2\pi \int_{\pi/2}^{\pi} \sigma(\theta) \sin \theta d\theta \quad (13)$$

where  $\sigma(\theta)$  is the differential cross section.

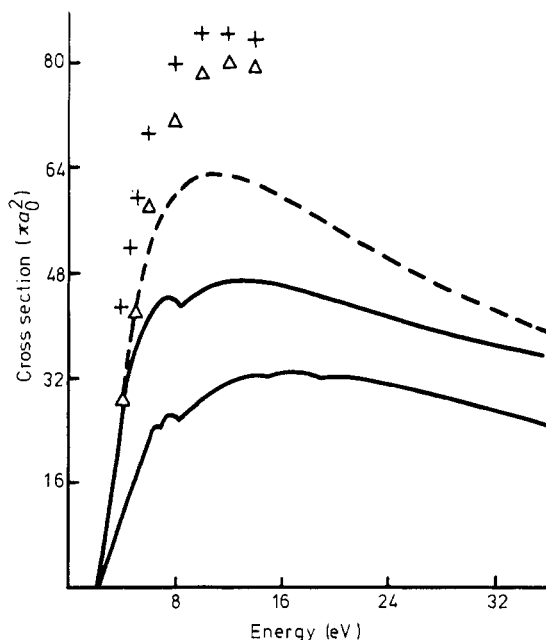
**Table 1.** Integral cross sections for elastic scattering by Ba atoms (in units  $\pi a_0^2$ ).

$E(\text{eV})$	6	7	8	10	14	20	24	30	35
$Q$	60.8	53.1	47.6	41.7	36.9	36.2	35.5	34.4	33.5
$Q_h$	10.1	9.4	9.0	8.3	6.2	5.2	4.3	3.0	2.1
$Q_{\text{exp}}$	—	—	—	—	—	68.9	—	41.3	—

$Q_h$  are the cross sections for scattering in the back hemisphere (13).  $Q_{\text{exp}}$  are the experimental values of Jensen *et al* (1978).

It should be noted that when energy varies from 20 to 30 eV, the variation of the theoretical cross section is very small, while an experimental cross section varies significantly. This disagreement is probably caused by the difficulties in extrapolation mentioned above.

The integral excitation cross sections for Ba are shown in figure 3. Results of calculations with parameter  $c = 1$  (equation (3)) in  $6^1\text{S}-6^1\text{P}$  and  $6^1\text{S}-6^1\text{P}-5^1\text{D}$  approximations  $5^1\text{D}$  being included without exchange are also given. Weak influence of the  $5^1\text{D}$  level on the results is seen for  $E > 8$  eV. Disagreement with the data of Chen and Gallagher (1976) is largest in the region of the cross section maximum where the theoretical cross section exceeds the experimental one by over 34%. At higher energies the theoretical curve approaches Chen and Gallagher's curve. This fact seems to point



**Figure 3.** Integral cross sections for excitation of the Ba resonance line. Full curves 1 and 2 are the experimental results of Aleksakhin *et al* (1975) and Chen and Gallagher (1976) respectively. The broken curve is the result of close-coupling calculations with the parameter  $c = 0.809$  in formula (3). The points are:  $6^1\text{S}-6^1\text{P}-5^1\text{D}$  close-coupling calculations with  $c = 1$  ( $5^1\text{D}$  level included without account of exchange); +, similar calculations with including of  $6^1\text{S}-6^1\text{P}$  coupling.

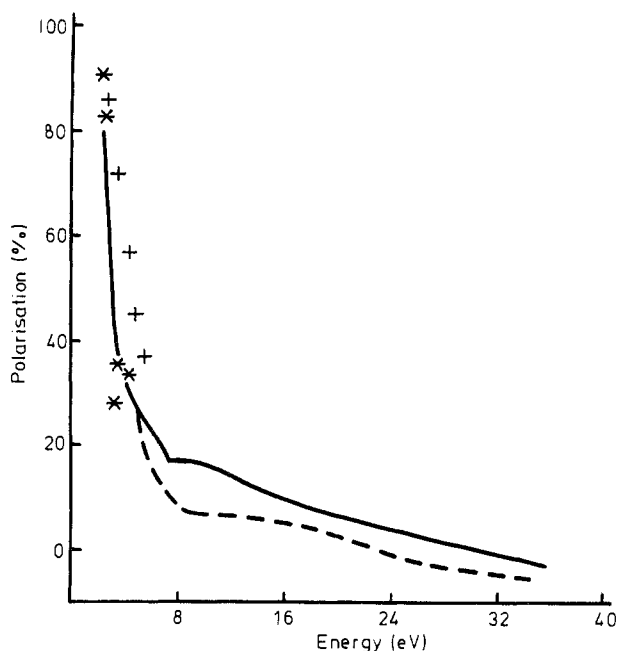
to the significance of the configuration interaction and core polarisation in the region of the maximum.

Disagreement between the data of Aleksakhin *et al* (1975) and Chen and Gallagher (1976) is caused by a substantial error in the first experiment (40%) and by a cascade contribution to the Chen and Gallagher cross sections. New data presented by Starodub (1976) are obtained with the account of the re-absorption of the resonance radiation in the atomic beam. The magnitude of Starodub's cross section is 37% higher than that obtained by Aleksakhin *et al* (1975). New results for  $E > 15$  eV actually coincide with the data of Chen and Gallagher.

Note that the theoretical curve has no structure at  $E \approx 8$  eV which was found by Aleksakhin *et al* (1975) and Chen and Gallagher (1976). This structure is caused either by cascade transitions or by the coupling neglected in our calculations.

Data on the polarisation of the Ba resonance line are presented in figure 4. Good agreement with Chen and Gallagher's results is observed at  $E < 5$  eV (with the exception of  $E = 3$  eV where the theoretical polarisation is too low (28.4%)). For higher energies theoretical and experimental results diverge and begin to converge slowly at  $E \geq 20$  eV.

In table 2 integral cross sections for Mg are listed and a comparison with other calculations and experimental data is presented. Disagreement between the calculations and experimental data of Leep and Gallagher (1976) at the maximum of the cross section ( $E \approx 20$  eV) is approximately the same as for Ba. It seems that in this case, exchange between the incident electron and atomic core electrons is also important.



**Figure 4.** Polarisation of the Ba resonance line. The full curve represents the experimental results of Chen and Gallagher (1976). The broken curve and \* are the results of the  $6^1S-6^3P$  close-coupling calculations with  $c = 0.809$ . Crosses, +, are  $6^1S-6^3P-6^1P$  close-coupling calculations with  $c = 1$ , i.e. the results of the previous paper (Fabrikant 1975) reconsidered taking into account the isotope mixture.



**Table 2.** Integral cross sections for elastic scattering and excitation of Mg atoms (in units  $\pi a_0^2$ ).

<i>E</i> (eV)		Experiment			Theory				
		a	b	c	d	e	f	g	h
10	elastic	32	—	—	29.0	—	—	—	—
	excitation	16	8.3	16.0	19.7	15.6	12.0	42.0	34.2
20	elastic	18	—	—	14.0	—	—	—	—
	excitation	17	9.6	17.3	24.3	—	—	—	30.7

<sup>a</sup> Williams and Trajmar (1978).<sup>b</sup> Aleksakhin *et al* (1973).<sup>c</sup> Leep and Gallagher (1976).<sup>d</sup> Present results.<sup>e</sup> Close-coupling calculations with Hartree-Fock atomic wavefunctions (Robb 1975).<sup>f</sup> The same calculations with configuration-integration functions (Robb 1975).<sup>g</sup> The Born approximation with configuration-interaction wavefunctions (Robb 1974).<sup>h</sup> The unitarised Born approximation with semi-empirical wavefunctions (Vainshtein *et al* 1973).

Indeed, the calculations of Robb (1975) carried out with Hartree-Fock atomic wavefunctions taking into account this exchange give the value of the cross section at 10 eV which is smaller than ours by  $4\pi a_0^2$ . Accurate account of the configuration interaction leads to the following drop in the cross section.

The results of the unitarised Born approximation (Vainshtein *et al* 1973) are quite close to the present data at 20 eV. (It is essential that in both calculations the same semi-empirical atomic wavefunctions were used.) For Ba the results of the unitarised Born approximation still exceed ours at  $E = 30$  eV by the factor of two.

For the polarisation of radiation (table 3) the agreement between the calculation and experimental data of Leep and Gallagher (1976) is much better than that for the cross sections. Calculations in the Born approximation (Robb 1974) also give values close to the experimental ones, since the Born approximation is better for relation (11) than for cross section  $Q = Q_0 + 2Q_1$  (Robb 1974).

**Table 3.** Polarisation of the Mg resonance line excited by electron impact.

<i>E</i> (eV)	Present results	Leep and Gallagher (1976)	Robb (1974)
10	52.4	47.4	53.0
20	22.1	23.3	—

### Acknowledgments

I should like to thank Dr I Yevlampiyev and Dr I Khinich for discussions, which stimulated the appearance of the present work and Dr V Starodub for comments concerning some aspects of his work.

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