Coupled-channels optical calculation of electron-magnesium scattering


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Coupled-channels optical calculation of electron–magnesium scattering

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Abstract. The coupled-channels optical method is used to study the electron–magnesium scattering process at intermediate energies. Continuum optical potentials were included in the calculations. Differential and total cross sections are reported for the elastic and inelastic (3lP and 33P) transitions at 10, 20 and 40 eV. The present calculations show fair agreement with experimental data for differential and total cross sections.

1. Introduction

In recent years the optical potential approach has been widely used in studying electron–atom reaction processes at intermediate energies (McCarthy and Stelbovics 1980, Bransden et al 1982, Callaway and Oza 1985, Bartschat et al 1988, Bray et al 1989a, b). In particular, the coupled-channels optical (cco) method of McCarthy and Stelbovics (1983) has done reasonably well in calculating elastic and inelastic differential cross sections for e–H scattering (Lower et al 1987). Their ab initio optical potential has now been extended to calculate electron scattering from two-electron atoms (McCarthy et al 1988).

The recent measurements of the differential cross sections for electron impact excitation of the 3lP state (Brunger et al 1988) and the 33P state (Houghton et al 1989) in magnesium have provided a much more discriminating set of data than that of Williams and Trajmar (1978). The recent five-state close-coupling calculation of Mitroy and McCarthy (1989) seems to agree fairly well with the elastic differential cross section data of Williams and Trajmar (1978) for small angles at 10, 20 and 40 eV. Furthermore, for the 3lP excitation, the theoretical results are in remarkably good agreement with the data of Brunger et al (1988) at 10 and 20 eV for all angles. At 40 eV, however, the agreement holds only for the forward angles (θ < 40°). For the middle and backward angles, the theory predicts larger cross sections than any of the experiments.

The subsequent measurements of the differential cross sections for the 33P excitation (Houghton et al 1989) and the parallel development of the optical potential for two-electron atoms has provided an opportunity to test the cco model.

In this paper we present the results of a six-state close-coupling calculation done on e–Mg scattering. The six-state basis includes the 33P state in addition to the five lowest singlet states used by Mitroy and McCarthy (1989). It consists of the 3lS, 3lP, 33P, 31D, 4lS and 41P states. The target states are represented by configuration interaction
(CI) wavefunctions as described by Mitroy and McCarthy (1989). The calculations were done in two models. In the CC6 model, no continuum optical potentials were included in the calculation. The CC06 model had the continuum optical potentials included in the $3^1S-3^1S$, $3^1S-3^1P$, $3^1P-3^3P$ and $3^1S-3^3P$ couplings. Optical potentials for discrete states outside the coupled space were not taken into account because the large basis set used in the present calculations accounts for most of the coupling to discrete states.

2. Coupled channels optical calculation

A detailed description of the coupled-channels optical method to study electron–atom scattering processes in momentum space can be found in McCarthy and Stelbovics (1983). The generalisation of the CCO method to allow for CI (configuration interaction) wavefunctions for the target states has been discussed by Bray et al (1989b). Here we briefly review the essential features of the CCO method.

The coupled-channels optical calculation involves the solution of the coupled integral equations (McCarthy and Stelbovics 1983)

$$\langle k | T | j k_j \rangle = \langle k | V + V^{(Q)} | j k_j \rangle + \sum_{\ell \in P} \int d^3 k \langle k | V + V^{(Q)} | l k \rangle (E^{(+)} - \epsilon_\ell - \frac{1}{2} k^2)^{-1} \langle k | T | j k_j \rangle$$

(1)

where

$$\langle k | T | j k_j \rangle = \langle k | V | \Psi^{(+)\ell}(k_j) \rangle$$

(2)

is the $T$-matrix element for the transition from the $(N + 1)$-electron channel state $| j k_j \rangle$ to $| i k_i \rangle$. The ket $| \Psi^{(+)\ell} \rangle$ is the formally exact solution of the $(N + 1)$-electron Schrödinger equation with total energy $E$ for entrance channel $j$ while $\epsilon_\ell$ is the energy of the $N$-electron target state $| j \rangle$. The first-order electron–target potential $V$ includes the appropriate exchange operator. The complex polarisation operator $V^{(Q)}$ is written in the Feshbach formalism as

$$V^{(Q)} = PVQ \left( \frac{1}{E^{(+)} - QHQ} \right) QVP$$

(3)

where the operators $P$ and $Q$ project the explicitly-coupled channels and the remaining channels respectively.

The optical potential matrix elements for two-electron target atoms can be written (in the notation of McCarthy et al 1988)

$$\langle k_{i,j} | V^{(Q)} | j k_j \rangle = \int d^3 k \sum_{i \in Q} (a_s + b_s P_i) \langle k_{i,j} | V | \Psi^{(-)\ell}_l(k) \rangle \times (E^{(+)} - \epsilon_\ell - \frac{1}{2} k^2)^{-1} \langle \Psi^{(-)\ell}_l(k) | V | j k_j \rangle.$$  

(4)

Here $\Psi^{(-)\ell}_l(k)$ is the three-body wavefunction for a final target state $l$ with the appropriate boundary conditions and $P_i$ is the space-exchange operator. The spin coefficients $a_s$ and $b_s$ which depend on the total spin $S$ are explicitly detailed in McCarthy et al (1988). For the continuum target states $l$ the summation is replaced by a momentum integration.
In the present work the $Q$-space considered includes the continuum channels only. Using the screening approximation (McCarthy and Stelbovics 1980) we write the continuum polarisation potential as

$$
\langle k_i | V^{(Q)} | j k_j \rangle = \int d^3 k' \int d^3 k (a_S + b_S P_r) \langle k_i | V | \varphi^{(-)}(k_<) | k_j \rangle
\times \left[ E^{(+)} - \frac{1}{2} (k^2 + k'^2) \right]^{-1} \langle k_< | \varphi^{(-)}(k_<) | V | j k_j \rangle
$$

(5)

where $\varphi^{(-)}(k_<)$ is the Coulomb wave (orthogonalised to the bound state from which the electron was excited) which represents the slower electron. For computational tractability, an angular momentum projection is used to approximate the non-local optical potential and $k_j$ is taken to be on the energy shell (McCarthy and Stelbovics 1980).

The angular momentum projection of the optical potential matrix element is

$$
V_{\ell' \ell'}(K) = \sum_{m' m} C_{n' m' m}^{\ell' \ell} \int d^K \langle k_i | V^{(Q)} | j k_j \rangle i^{-\ell'} Y_{\ell' m'}^* (\hat{K})
$$

(6)

where $K = k_j - k_i$, the orbital angular momentum quantum numbers $\ell'$, $m'$ and $l$, $m$ belong to the target states $i$ and $j$ respectively and $C_{n' m' m}^{\ell' \ell}$ denotes the Clebsch–Gordan coefficients. For the optical potential calculation the target states are represented by the appropriate Hartree–Fock configuration. The set of coupled integral equations (1) is solved following the numerical techniques as detailed by McCarthy and Stelbovics (1983).

3. Results and discussion

Elastic differential cross sections at energies of 10, 20 and 40 eV are depicted in figure 1. The present CC6 and CCO6 calculations are compared with the experimental data of Williams and Trajmar (1978). The previous CC5 calculation of Mitroy and McCarthy (1989) is also shown. Except for the middle and backward angles at 10 and 20 eV, the present calculations are quite similar to the CC5 calculation. The CCO6 calculation agrees better with the experimental data at small angles ($\theta < 40^\circ$) for all energies, although the forward peaks are slightly overestimated at 10 and 20 eV. The influence of the $3^3P$ state in the coupling seems to be important at 10 eV. This can be seen in table 1 where the total elastic cross section of the CC6 calculation is about 10% larger than the CC5. At 20 eV CC6 predicts a deeper minimum than CC5 and CCO6. It seems that use of the continuum polarisation potentials is best at 40 eV, where agreement between the CCO6 model and experiment is better than any other theoretical calculations done so far. The use of optical potentials seems to enhance the cross sections for the forward angles, thus giving larger total cross sections at all energies.

The theoretical differential cross sections for the $3^3P$ transition are compared with the experimental data of Brunger et al (1988) in figure 2. In general, the shapes predicted by the theory are in fair agreement with experiment. The inclusion of the $3^3P$ state shows some appreciable differences in the calculated differential cross sections. CC6 is in better agreement with the experimental data for small angles ($\theta < 50^\circ$) at 10, 20 and 40 eV compared with the CC5 model. For $\theta > 50^\circ$, at 10 and 20 eV, there are some interesting features of the comparison between the CC5 and CC6 calculations. At 10 eV, the CC6 backward angle cross sections are less sloping and larger than the
Figure 1. The differential cross section for elastic electron scattering on magnesium at 10, 20 and 40 eV. Experimental data are due to Williams and Trajmar (1978). Curves: full curve, CCO6; broken curve with long dashes, CCO6; broken curve with short dashes, CCS.

Table 1. Total elastic cross sections ($\pi a_0^2$). Experimental values quoted are from Williams and Trajmar (1978).

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>CCO6</th>
<th>CCO6</th>
<th>CCS</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>33.20</td>
<td>27.82</td>
<td>25.20</td>
<td>32.96</td>
</tr>
<tr>
<td>20</td>
<td>14.91</td>
<td>12.63</td>
<td>12.10</td>
<td>18.19</td>
</tr>
<tr>
<td>40</td>
<td>8.23</td>
<td>8.05</td>
<td>7.53</td>
<td>7.50</td>
</tr>
</tbody>
</table>

Figure 2. The differential cross section for the excitation of the $3^1P$ state of magnesium. Experimental data are due to Brunger et al (1988). Curves are as described for figure 1.

CCS, while at 20 eV we find the CCO6 cross sections are smaller and tend to be flat. These differences disappear at 40 eV. The CCO6 calculation agrees fairly well with the experimental data for small angles at 10 and 20 eV. For backward angles it tends to underestimate the cross sections. At 40 eV, we find the CCO6 model showing the best
Coupled-channels optical calculation of e–Mg scattering

Table 2. Total cross sections for electron excitation of the $^{3}\text{P}$ state of magnesium ($\pi a_0^2$).
Experimental values (with cascade contributions) are from Leep and Gallagher (1976). The asterisk denotes that cascade contributions have been included.

<table>
<thead>
<tr>
<th></th>
<th>10 eV</th>
<th>20 eV</th>
<th>40 eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>cco6</td>
<td>15.25</td>
<td>14.81</td>
<td>14.21</td>
</tr>
<tr>
<td>cc6</td>
<td>15.76</td>
<td>18.50</td>
<td>15.79</td>
</tr>
<tr>
<td>cc5</td>
<td>16.90</td>
<td>18.60</td>
<td>15.50</td>
</tr>
<tr>
<td>cco6*</td>
<td>19.34</td>
<td>17.63</td>
<td>16.10</td>
</tr>
<tr>
<td>cc6*</td>
<td>19.01</td>
<td>21.46</td>
<td>18.01</td>
</tr>
<tr>
<td>cc5*</td>
<td>20.20</td>
<td>21.30</td>
<td>17.40</td>
</tr>
<tr>
<td>Experiment</td>
<td>16.00</td>
<td>17.30</td>
<td>15.70</td>
</tr>
</tbody>
</table>

agreement with experiment of all the calculations.

In table 2 the total cross sections for the excitation of the $^{3}\text{P}$ state of magnesium calculated by the theoretical models are presented and compared with the experimental values of Leep and Gallagher (1976). Cascade contributions from the $4\text{S}$, $4\text{P}$ and $3\text{D}$ states are included using the formula (Mitroy and McCarthy 1989)

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

As expected, the present calculations show better agreement than the CCS model. The CCO6 cross section (with cascade contributions) is in good agreement with the experimental data of Leep and Gallagher at 20 and 40 eV. At 10 eV CCO6 and CCS6 are in fair agreement with the experimental cross section.

![Figure 3](image)

**Figure 3.** The differential cross section for the excitation of the $^{3}\text{P}$ state of magnesium. Experimental data: full circles, Houghton et al (1989); crosses, Williams and Trajmar (1978). Curves: full curve, CCO6; broken curve, CCO6; chain curve, two-configuration FOMBT (Meneses et al 1987a, b).

The experimental and theoretical differential cross sections for the $^{3}\text{P}$ state transition are depicted in figure 3. The CCO6 and CCS6 calculations seem to predict the general shape of the measured differential cross sections. At 10 eV, there is good...
agreement between the CCO6 and the experimental data of Houghton et al (1989). CCO6 underestimates the forward angle cross sections ($\theta < 40^\circ$) and predicts a minimum at around $110^\circ$. The experimental minimum is at about $120^\circ$. At 20 eV CCO6 shows fair agreement with experiment for forward angles while at backward angles ($\theta > 90^\circ$) it overestimates the cross section. CCO6 does slightly better at backward angles. The experimental data of Houghton et al (1989) show a backward peak at $110^\circ$. The present close-coupling calculations and the first-order many-body theory (FOMBT) calculation of Meneses et al (1987b) also predict a backward minimum at around $120^\circ$. It seems both theoretical models overestimate the backward peak. At 40 eV, the experimental data of Williams and Trajmar (1978) do not provide a good resolution to compare with the present results. Over the whole angular range, the CCO6 and CCO6 models give a similar shape. The CCO6 cross sections are slightly larger at all angles except at the minimum. For comparison, we also show the FOMBT values of Meneses et al (1987a) at 40 eV. Although the shapes predicted by the FOMBT and the coupled-channels method are quite similar there are some differences. At the forward angle ($\theta = 0$) and the backward angles ($\theta > 60^\circ$) FOMBT cross sections are larger than CCO6. Both theoretical models agree in the predictions of all maxima and minima.

Table 3. Integral cross sections ($\pi a_0^2$) for the electron excitation of the $3^3P$ state of magnesium. HTBS and WT denote the experimental values of Houghton et al (1989) and Williams and Trajmar (1978) and FOMBT denotes the first-order many-body theoretical calculation of Meneses et al (1987a, b).

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>HTBS</th>
<th>WT</th>
<th>FOMBT</th>
<th>CCO6</th>
<th>CCO6</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>3.22</td>
<td>3.52</td>
<td>4.31</td>
<td>4.13</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>0.58</td>
<td>0.91</td>
<td>0.56</td>
<td>0.69</td>
<td>0.76</td>
</tr>
<tr>
<td>40</td>
<td></td>
<td>0.034</td>
<td>0.093</td>
<td>0.063</td>
<td></td>
</tr>
</tbody>
</table>

The total cross section for the excitation of the $3^3P$ state of magnesium is given in table 3 for the present calculations together with the experimental data of Houghton et al (1989) and Williams and Trajmar (1978). The FOMBT calculation of Meneses et al (1987a) is also given. The present values show only fair agreement with experiment at 10 and 20 eV. At 40 eV it is difficult to draw any conclusions from the only available data of Williams and Trajmar (1978). It is interesting to note that the FOMBT value shows remarkable agreement with the data of Houghton et al (1989) at 20 eV, even though the differential cross sections (see figure 3) do not reflect that agreement.

Table 4. Total ionisation cross sections ($\pi a_0^2$) for magnesium. Experimental values were read from the published curves of Karstensen and Schneider (1975).

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>CCO6</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>3.84</td>
<td>5.91</td>
</tr>
<tr>
<td>20</td>
<td>7.32</td>
<td>7.28</td>
</tr>
<tr>
<td>40</td>
<td>4.83</td>
<td>4.66</td>
</tr>
</tbody>
</table>

In table 4, we compare the total ionisation cross sections calculated by the CCO6 model with the experimental ionisation cross sections of Karstensen and Schneider (1975). There is very good agreement between the CCO6 values and experiment. This is
an excellent indication of the validity of the optical potential in the treatment of the ionisation continuum.

4. Conclusions

The present work takes into account all effects in electron–atom scattering in approximations that have proved fairly good in other contexts. The target states are treated by moderately large configuration interaction expansions that are semiquantitatively successful in describing energies and oscillator strengths (Mitroy and McCarthy 1989).

Coupling of the six lowest-energy states of magnesium is treated exactly. Coupling to the continuum is treated by a half-on-shell approximation to the optical potential that has had semiquantitative success for hydrogen (Lower et al 1987) and helium (McCarthy et al 1988). Its first requirement, that it produces correct total ionisation cross sections, is well satisfied. The continuum for magnesium has a larger effect than for sodium (McCarthy et al 1985), where it was essentially negligible. The approximations made in the optical potential are expected to be more valid at higher energies.

Inclusion of the optical potential (CCO6) generally improves total and differential cross sections in comparison with pure close coupling (CC6). Total cross sections and trends in differential cross sections are described fairly well, but discrepancies between theory and experiment for large-angle differential cross sections are significant.

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