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A theoretical study of fast electron–helium scattering

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Abstract. The second order diagonalization method with a twenty two states basis (1^1S to 5^1D) is used to study electron–helium scattering. Our differential cross sections for the excitation of the $n = 2$ levels reproduce fairly well the experimental data up to large angles (60° or more) at energies above 50 eV. Our total cross sections for the 1^1S–n^1S and 1^1S–n^1D transitions ($n = 3, 4, 5$) are also in good agreement with experiment and improve greatly the first and second order Born results. The agreement between our 1^1S–n^1P cross sections and experiment is satisfactory only above 150 eV. The polarization of the 3^1P–2^1S and 3^1D–2^1P lines are also calculated and are in relatively good agreement with the experimental data.

1. Introduction

In three preceeding papers, we have studied proton and electron atomic hydrogen scattering (Baye and Heenen 1973a and 1974) and proton helium scattering (Baye and Heenen 1973b). We now complete our work and study electron helium scattering. The interest of this collision is a great amount of experimental data which is available and which allows a very fruitful comparison between theory and experiment, even for the $n = 2$ levels which were very poor in experimental data in proton helium scattering.

In § 2, we briefly give some basic formulae. In § 3, we compare various theoretical results with experiment for the differential and total 1^1S–2^1S and 1^1S–2^1P cross sections. Finally, we compare our results for higher levels and for polarizations with the Born approximation and with experiment.

2. Theory

We study the collision between a fast charged particle and a target with a Coulomb interaction between target and projectile. The transition amplitude from the ground state $|\mathrm{o}\rangle$ to a final state $|\mathrm{p}\rangle$ is given by (Byron 1971):

$$T_{\mathrm{po}} = \frac{k_{\mathrm{i}}}{2\pi \mathrm{i}} \int \mathrm{e}^{\mathrm{i}(\boldsymbol{k}_{\mathrm{i}} - \boldsymbol{k}_{\mathrm{f}}).\boldsymbol{b}} a_{\mathrm{po}}(\boldsymbol{b})\, \mathrm{d}\boldsymbol{b}$$

where $\boldsymbol{k}_{\mathrm{i}}$ and $\boldsymbol{k}_{\mathrm{f}}$ are the initial and final wavevectors of the projectile and b is the impact parameter. $a_{\mathrm{po}}(\boldsymbol{b})$ is the transition probability for the o to p transition. We calculate it by use of the second order diagonalization method (Baye and Heenen 1973a). To describe helium, we use the wavefunctions of configuration interaction type determined by Vanderpoorten (1973).

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We have chosen a trajectory along the z axis which makes the eikonal impact parameter form of the first Born approximation equivalent to the quantum first Born approximation (Baye and Heenen 1974). In this frame, we have, if $|p\rangle$ is a final state of magnetic quantum number m:

$$T_{\rm po} = -{\rm i}k_{\rm i}\int_0^\infty J_m\left[qb\left(1-\frac{(E_{\rm p}-E_{\rm o})^2}{q^2k_{\rm i}^2}\right)^{1/2}\right]a_{\rm po}(b)b\,{\rm d}b$$

where

$$\boldsymbol{q} = \boldsymbol{k}_{\rm i}-\boldsymbol{k}_{\rm f}$$

and $E_{\rm o}$ and $E_{\rm p}$ are the energies of initial and final states. The differential cross sections are related to $T_{\rm po}$ by:

$$\frac{{\rm d}\sigma_{\rm po}}{{\rm d}\Omega} = \frac{k_{\rm f}}{k_{\rm i}}|T_{\rm po}|^2.$$

The total cross sections are determined by integration of the differential cross sections.

3. Results

We show in table 1 the total cross sections that we have obtained with a 22 states basis.

Table 1. Total cross sections (in units of πa_0^2) obtained to the second order diagonalization method with a 22 states basis

E (eV)	50	100	200	400	1000
2^1S	0.198^{-1}†	0.150^{-1}	0.923^{-2}	0.529^{-2}	0.244^{-2}
2^1P$_0$	0.108	0.636^{-1}	0.355^{-1}	0.194^{-1}	0.898^{-2}
2^1P$_1$	0.862^{-1}	0.819^{-1}	0.649^{-1}	0.460^{-1}	0.261^{-1}
3^1S	0.346^{-2}	0.271^{-2}	0.174^{-1}	0.105^{-2}	0.516^{-3}
3^1P$_0$	0.300^{-1}	0.171^{-1}	0.901^{-2}	0.471^{-2}	0.222^{-2}
3^1P$_1$	0.215^{-1}	0.212^{-1}	0.168^{-1}	0.117^{-1}	0.646^{-2}
3^1D$_0$	0.140^{-2}	0.410^{-3}	0.157^{-3}	0.723^{-4}	0.310^{-4}
3^1D$_1$	0.105^{-2}	0.525^{-3}	0.220^{-3}	0.850^{-4}	0.181^{-4}
3^1D$_2$	0.328^{-3}	0.347^{-3}	0.262^{-3}	0.169^{-3}	0.847^{-4}
4^1S	0.109^{-2}	0.918^{-3}	0.613^{-3}	0.379^{-3}	0.192^{-3}
4^1P$_0$	0.119^{-1}	0.709^{-2}	0.377^{-3}	0.195^{-2}	0.910^{-4}
4^1P$_1$	0.806^{-2}	0.850^{-2}	0.691^{-2}	0.488^{-2}	0.266^{-2}
4^1D$_0$	0.650^{-3}	0.209^{-3}	0.869^{-4}	0.415^{-4}	0.174^{-4}
4^1D$_1$	0.569^{-3}	0.267^{-3}	0.102^{-3}	0.370^{-4}	0.800^{-5}
4^1D$_2$	0.185^{-3}	0.196^{-3}	0.147^{-3}	0.918^{-4}	0.453^{-4}
5^1S	0.426^{-3}	0.416^{-3}	0.293^{-3}	0.186^{-3}	0.940^{-4}
5^1P$_0$	0.502^{-2}	0.337^{-2}	0.187^{-2}	0.985^{-3}	0.454^{-3}
5^1P$_1$	0.326^{-1}	0.384^{-2}	0.332^{-2}	0.241^{-2}	0.132^{-2}
5^1D$_0$	0.271^{-3}	0.117^{-3}	0.536^{-4}	0.256^{-4}	0.103^{-4}
5^1D$_1$	0.212^{-3}	0.108^{-3}	0.431^{-4}	0.157^{-4}	0.370^{-5}
5^1D$_2$	0.184^{-3}	0.130^{-3}	0.867^{-4}	0.525^{-4}	0.252^{-4}

† The superscript denotes the power of ten by which the number must be multiplied.

3.1. $n = 2$ levels

3.1.1. Differential cross sections. We compare in figure 1 various theoretical and experimental results for the 1^1S–2^1S transition at 100 eV.

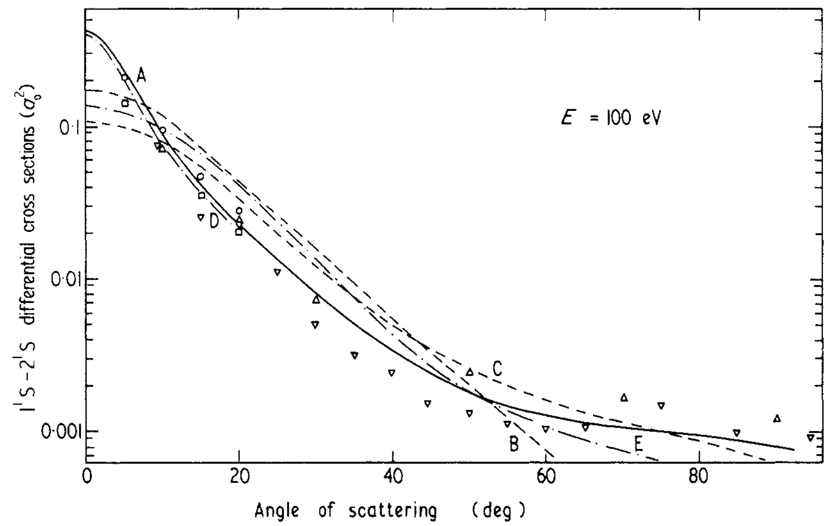

Figure 1. Differential cross sections for the 2^1S excitation of helium by electrons at 100 eV. Curve A our results; curve B first Born approximation; curve C distorted wave approximation of Joachain and Vanderpoorten (1974); curve D four channel results of Berrington *et al* (1973); curve E Hidalgo and Geltman (1972); ○ Vriens *et al* (1968); □ Vriens *et al* (1968) renormalized to Chamberlain *et al* (1970) at 5°; △ Crooks and Rudd (1972); ▽ Suzuki and Takayanagi (1973); × Opal and Beaty (1972); + Rice *et al* (1972).

The differential cross sections obtained by Berrington *et al* (1973) at small angles using the method of Bransden *et al* (1972) are smaller than ours but show the same angular functional dependence. The distorted wave results of Joachain and Vanderpoorten (1974) who use the Glauber potential as distorted potential do not show the same forward peak as do our results. We also show the cross sections obtained by Hidalgo and Geltman (1972), which seem to be too low at large angles. Our results are in good agreement with experiments.

We show in figure 2 the differential cross sections for the 1^1S–2^1S transition at various energies.

Our values at 5° are, below 400 eV, in better agreement with the values of Vriens *et al* (1968) than with those obtained by Chamberlain *et al* (1970). All the experimental results normalized to Chamberlain's ones at 5° are therefore lower than ours. Nevertheless, the agreement between our theoretical results and experiment is good up to large scattering angles above 100 eV. At 81·63 eV, the agreement is good with the values of Rice *et al* (1972) renormalized to ours at 8° but there is no agreement with the data of Opal and Beaty (1972). At 50 eV, the agreement with the values of Crooks and Rudd (1972) is satisfactory only up to 60°.

The results of the second order Born approximation obtained by Holt *et al* (1971) and by Woollings and McDowell (1972) are not in agreement with ours below 400 eV.

We display in figure 3 the differential cross sections for the 1^1S–2^1P transition.

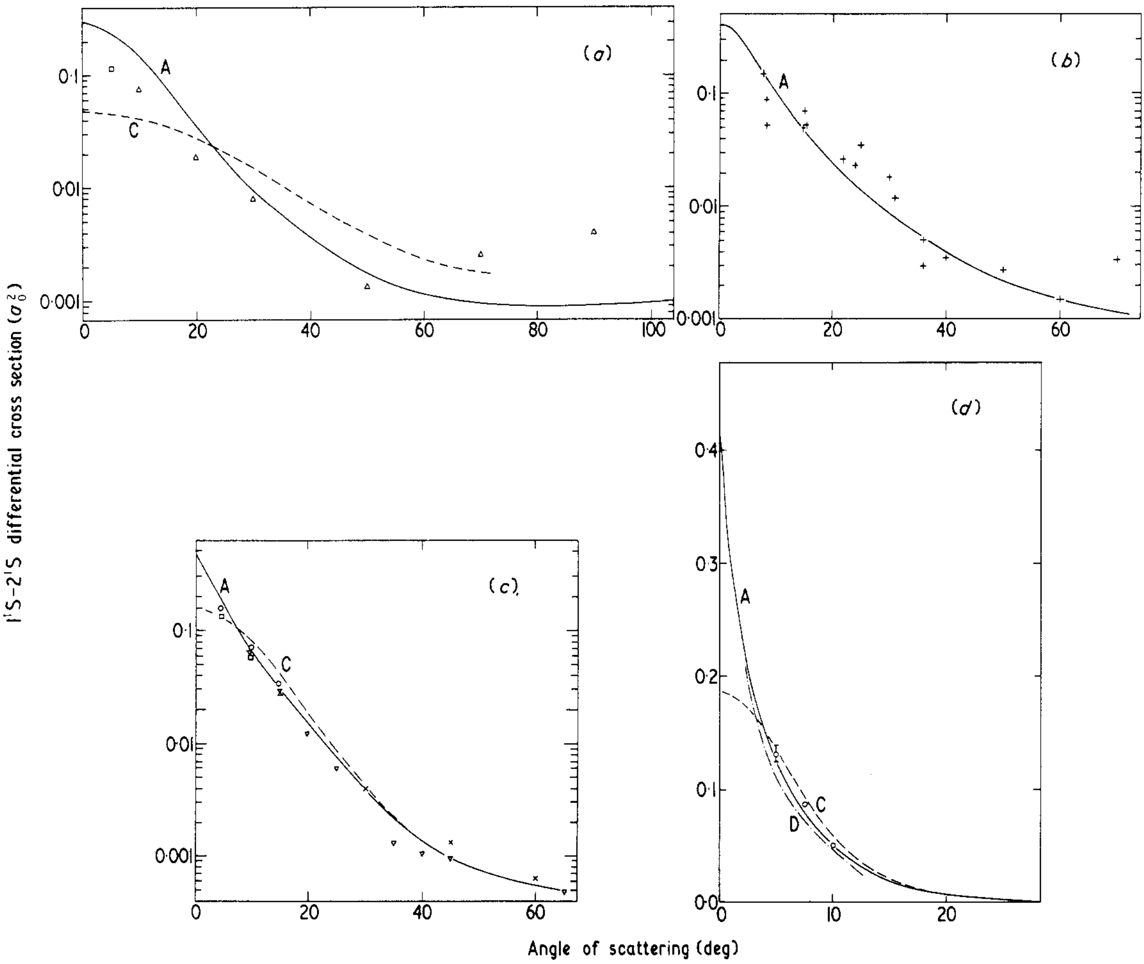

Figure 2. Differential cross sections for the 2^1S excitation of helium by electrons at (*a*) 50 eV (*b*) 81·63 eV (*c*) 200 eV and (*d*) 400 eV. Same notations as figure 1.

At 50 eV, we have renormalized the values obtained by Truhlar *et al* (1970) and by Crooks and Rudd at our values at 10°.

The agreement of our cross sections with experiment is very good up to large scattering angles, except at 50 eV where there is no agreement above 60° and at 81·63 eV with the measurements of Opal and Beaty (1972).

Our cross sections are also in good agreement with the calculations at small angles by Berringtom *et al* (1972) and by Woollings and McDowell (1972) at 200 eV. Our results also show the same behaviour as those of Hidalgo and Geltman (1972) for large angles but are lower by almost a factor 2 at small angles.

We do not show the distorted wave results of Madison and Shelton (1972). Some of the cross sections which they obtained seem to have a correct behaviour up to very large scattering angles, but it does not seem to be a criterion for choosing between the various curves proposed by these authors.

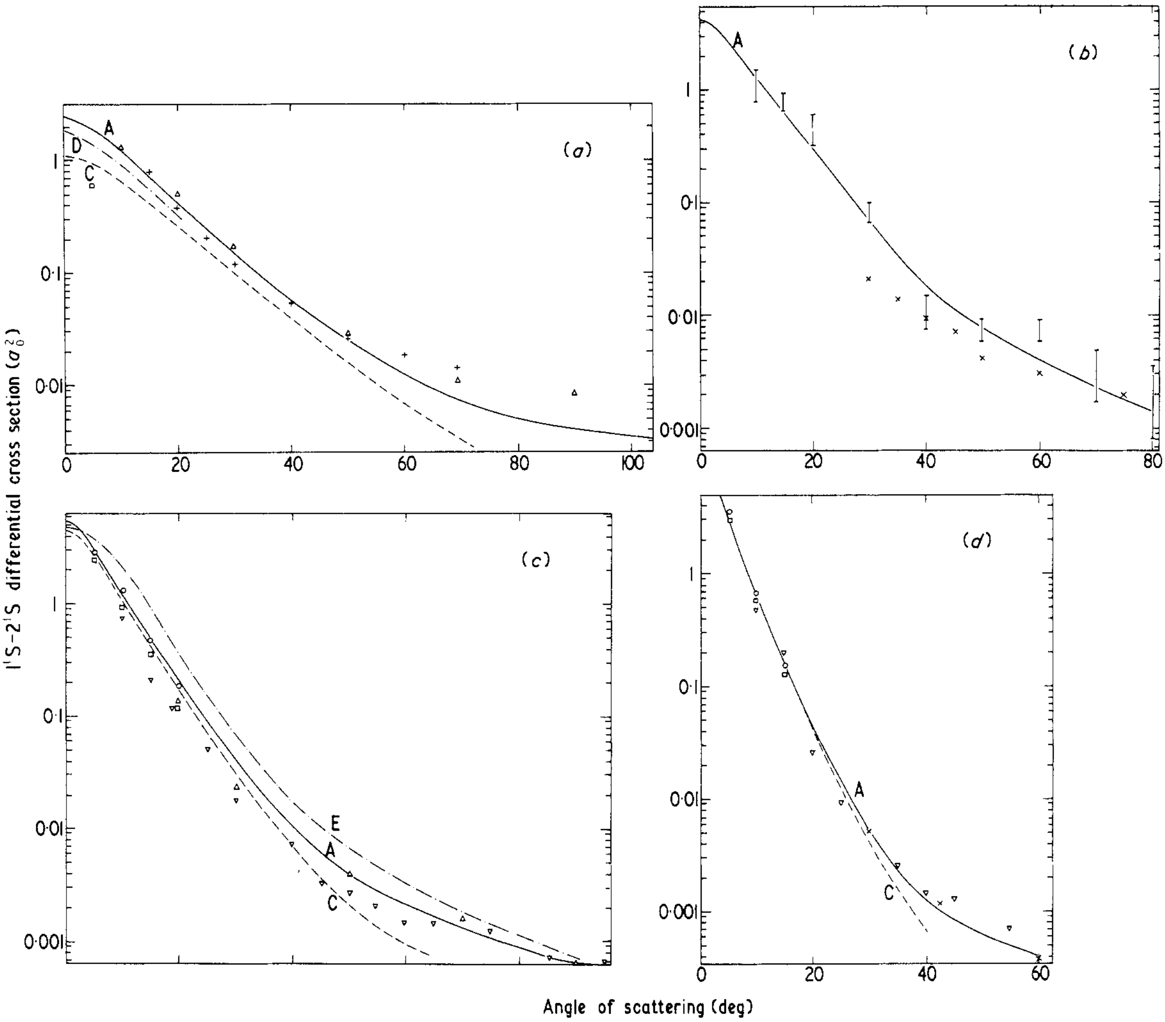

Figure 3. Differential cross section for the 2^1P excitation of helium by electrons at (*a*) 50 eV (*b*) 81·6 eV (*c*) 100 eV (*d*) 200 eV. Same notations as figure 1 except Ｉ Truhlar *et al* (1970).

3.1.2. Total cross sections. We display in figure 4 the total 1^1S–2^1S cross sections.

Our cross sections are in good agreement with those of Joachain and Vanderpoorten (1973) and of Berrington *et al* (1973) above 100 eV and are lower than the first order (Bell *et al* 1969) and second order (Woollings and McDowell 1972) Born results. The agreement with the experimental data is satisfactory.

We show in figure 5 the total 1^1S–2^1P cross sections.

We have renormalized the experimental results of Donaldson *et al* (1972) within their estimated error in absolute magnitude.

The results of Berrington *et al* (1973) are almost identical to ours at all energies. Both overestimate the cross sections at low energies and are in agreement with experiment only above 100 eV while the cross sections obtained by Joachain and Vanderpoorten (1974) are in close agreement with the experiment of Donaldson.

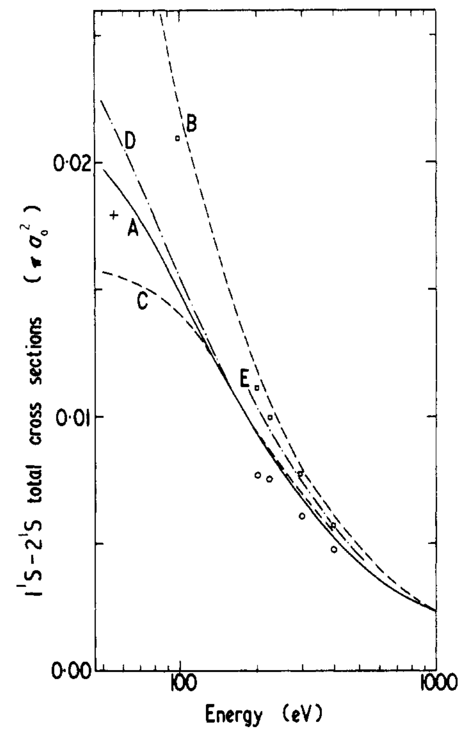

Figure 4. Total cross sections for the 2^1S excitation of helium by electrons. Same notations as in figure 1 except curve E second Born approximation (Woollings and McDowell 1972); □ Lassettre *et al* (1967).

The cross sections obtained by Flannery (1970) are not shown in these two figures and are in good agreement with our values for the $1^1S–2^1P$ cross sections and with the second Born values for the $1^1S–2^1S$ cross sections.

3.2. $n > 2$ levels

As it has been pointed out by Thomas (1972) in proton helium scattering, the main source of error in the comparison between theory and experiment is the uncertainty on the normalization of experiment. In order to eliminate this error, we have normalized the experimental values to our values at the highest energy used in the comparison (in all cases 1 keV). This normalization of the experiment has also the advantage to eliminate the smaller error due to the helium wavefunctions we use. (The Born cross sections calculated with these wavefunctions are more accurate than 5 %–Vanderpoorten 1973).

One experimental group (Donaldson *et al* 1972) has given an estimated error due to the normalization: our normalization of their measurement is always within this error and is therefore fully justified. For another group (Van Raan *et al* 1971), the normalization factor is almost constant for all the transitions studied (it varies from 0·78 to 0·85). This may indicate a light systematic normalization error of the experience.

3.2.1. n^1S states. We show in figure 6 the $1^1S–n^1S$ cross sections multiplied by the energy for $n = 3, 4, 5$. One can see that our method is a great improvement on the

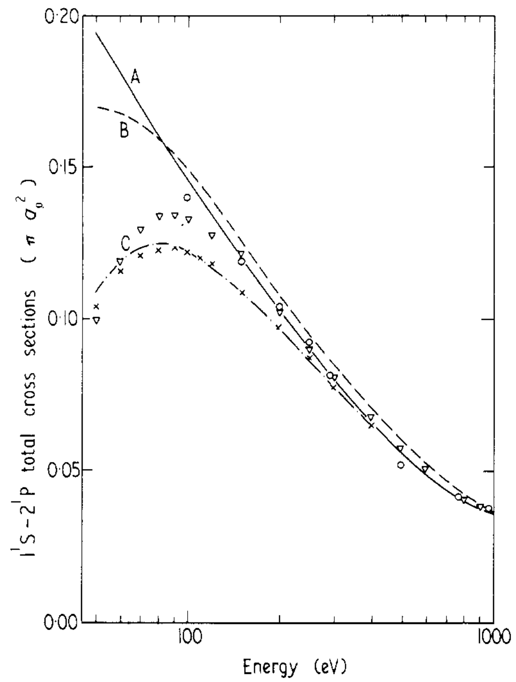

Figure 5. Total cross sections for the 2^1P excitation of helium by electrons. Same notations as in figure 1 except: ▽ Van Eck and de Jongh (1970); × Donaldson *et al* (1972).

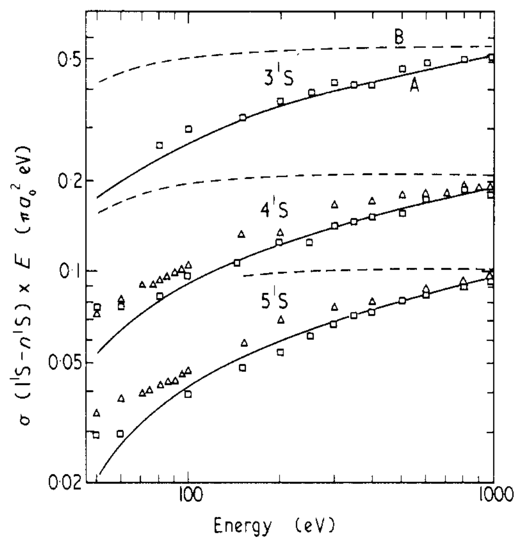

Figure 6. Total cross sections for the n^1S excitation of helium by electrons. Curve A our results; curve B first Born approximation; □ Moustafa Moussa *et al* (1969); △ Van Raan *et al* (1971).

first Born approximation. Our results for the three states are in very good agreement with the experiment of Moustafa Moussa *et al* (1969) and of Van Raan *et al* (1971) from 50 eV up to high energies, while the Born approximation overestimates the cross sections at low energies.

3.2.2. n^1P states. We display in figure 7 the 1^1S–n^1P cross sections multiplied by the energy for $n = 3, 4, 5$. The agreement with experiment is good only above 150 eV. In this region, the agreement with the first Born approximation is also good, and our method does not yield any improvement on the first Born results at energies below 150 eV. This is rather surprising, because there was a close agreement between our results and experiment in proton helium scattering (Baye and Heenen 1973b). The discrepancy in the electron case must be due to quantum effects not correctly treated in our impact parameter method.

The experimental data of de Jongh and Van Eck (1971) obtained with their third method are in relatively good agreement with the other measurements above 100 eV. For clarity, these are not shown in the figure.

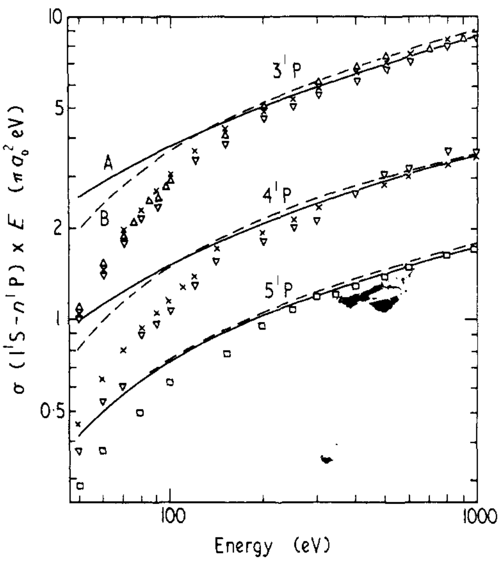

Figure 7. Total cross sections for the n^1P excitation of helium by electrons. Same notations as in figure 6 with: × Donaldson *et al* (1972); ▽ Van Eck and de Jongh (1970).

3.2.3. n^1D and 4^1F states. We show in figure 8 the 1^1S–n^1D cross sections times energy for $n = 3, 4, 5$. Again, our method is a great improvement on the Born approximation. The agreement between the second order diagonalization method and experiment is good while the first Born cross sections do not have the right behaviour up to very high energies. The second order Born results of Woollings and McDowell (1973) are smaller than the first Born results and do not have the right functional dependence in energy. These authors suggest to normalize the experiment to Born at 1 keV but our results indicate that this energy is not high enough.

We compare in table 2 our results for 1^1S–3^1D and 1^1S–4^1F cross sections with the experiment of Anderson *et al* (1969). There is no agreement in spite of the very large experimental errors reported by Anderson. We must notice that there is also no agreement between the 100 eV measurement by Moustafa Moussa *et al* (1969) and by Anderson.

We show in figure 9 differential cross sections for the 1^1S–3^1D transition at 400 eV and 200 eV.

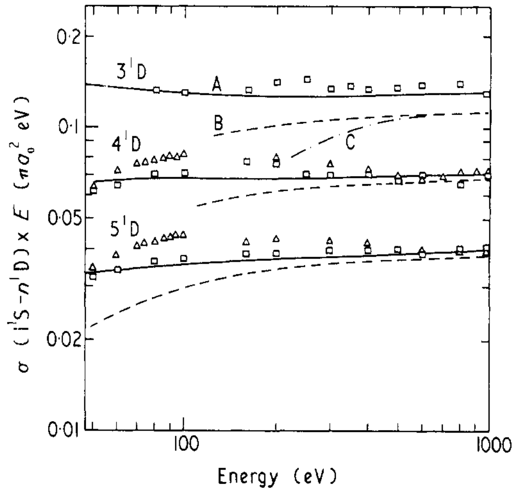

Figure 8. Total cross sections for the n^1D excitation of helium by electrons. Same notations as in figure 6 with: C second Born approximation (Woollings and McDowell 1973).

Table 2. Comparison between the experimental cross sections of Anderson *et al* (1969) and our values (in units of $10^{-3}\pi a_0^2$) for the excitation of the 3^1D and 4^1F states. The 4^1F results are obtained with a 20 states basis

E (eV)	3^1D		4^1F	
	Theory	Experiment	Theory	Experiment
50	2·78	$4·44 \pm 0·46$		
100	1·28	$2·62 \pm 0·34$	0·017	$0·126 \pm 0·063$

Our results have a very different behaviour from the first and second Born results of Woollings and McDowell. We find a larger forward peak and a very different decrease.

3.3. Polarization

We display in figure 10 the polarization of the 3^1P–2^1S line.

The agreement between our results and experiment is satisfactory in all the energy range studied. We are in better agreement at low energies with the recent experiment of Mumma *et al* (1973) than with the values obtained by the other experimental groups.

The polarizations that we have found for the 4^1P– and 5^1P–2^1S lines are almost identical to the 3^1P–2^1S polarizations. There is no agreement for these lines with the experiments of Moustafa Moussa *et al* (1969) who found that these lines are almost unpolarized.

We show in figure 11 the polarization of the 3^1D–2^1P line.

The agreement between our values and experiment is not very good, but, as in the proton helium case (Baye and Heenen 1973b) our results improve the first Born approximation.

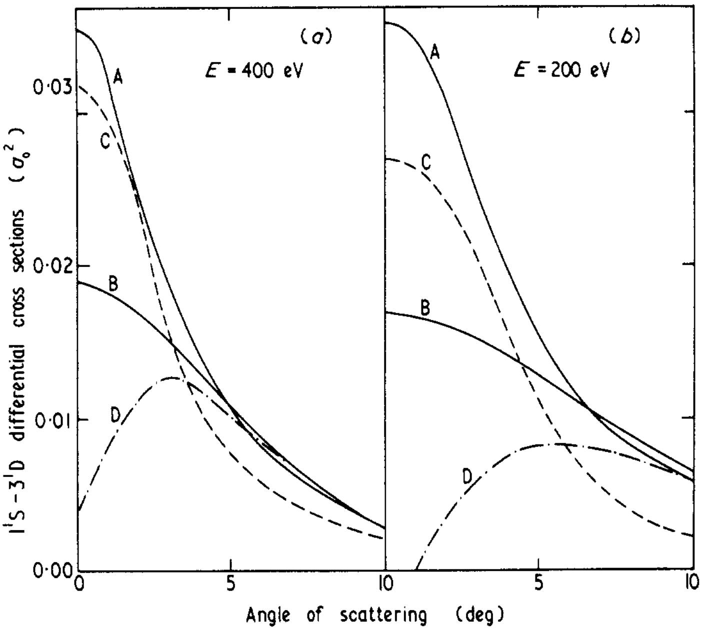

Figure 9. Differential cross sections for the 3^1D excitation of helium by electrons at (*a*) 400 eV and (*b*) 200 eV. Curve A our results; curve B first Born approximation; curve C second Born: W McD approximation (Woollings and McDowell 1973); curve D second Born: HM approximation (Woollings and McDowell 1973).

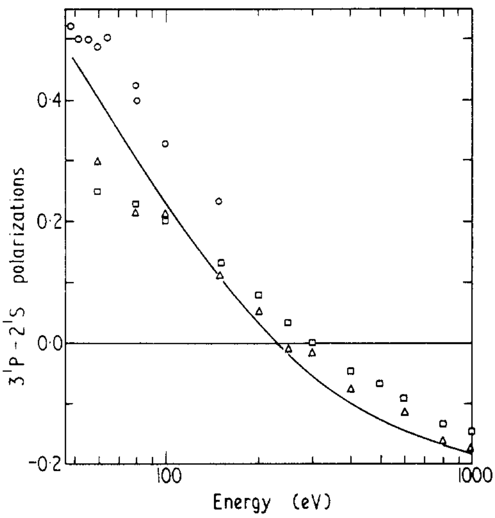

Figure 10. Polarization of the 3^1P–2^1S line. Same notations as in figure 6 with: ○ Mumma *et al* (1973).

4. Conclusion

The second order diagonalization method gives very good results for most of the cross sections and polarizations calculated in this paper for energies larger than 50 eV. The

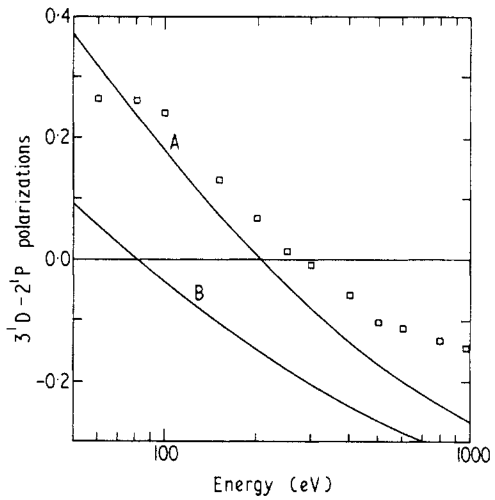

Figure 11. Polarization of the $3^1D–2^1P$ line. Same notations as in figure 6.

$1^1S–n^1D$ cross sections and the $^1D–^1P$ polarizations are in much better agreement with the experimental data than first and second Born calculations. However, our $1^1S–n^1P$ cross sections seem to be too large at energies below 150 eV.

Our differential cross sections reproduce fairly well the experimental data for angles below 60 degrees. For larger angles, our results are in better qualitative agreement than the other theoretical results. For very small angles the theoretical differential cross sections behave often quite differently but no experiment is available to compare with.

We have shown for proton collisions (Baye and Heenen 1973a and b) that the diagonalization method is a good approximation of the close-coupling method but allows the use of a larger number of states. We can conclude from the present paper that approximations related to the close coupling method give also good results for electron collisions, in the energy range where the eikonal approximation is valid and where the exchange effects are negligible. Both conditions seem to be well fulfilled in electron–helium scattering (except probably for the $1^1S–n^1P$ transitions at low energies).

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