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The use of second order potentials in the theory of the scattering of charged particles by atoms
IV. Electron scattering of helium atoms

K A Berrington†, B H Bransden† and J P Coleman‡
‡Department of Mathematics, †Department of Physics, University of Durham, England

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Abstract. The method of paper I is applied to the scattering by helium atoms of electrons between 50 and 1000 eV, and results are presented for elastic scattering and the 2^1S and 2^1P excitation. It is found that the inclusion of second order potential terms leads to cross sections which are in significantly better agreement with the experimental data than those of previous calculations.

1. Introduction

In paper I of this series (Bransden and Coleman 1972) a truncated eigenfunction expansion method for atomic collisions was described in which allowance was made for the effect of states not explicitly included in the expansion. This was successfully applied in papers II (Bransden *et al* 1972) and III (Sullivan *et al* 1972) to the scattering of electrons and protons from hydrogen atoms. In this paper we apply the same methods, again in the impact parameter formulation, to elastic scattering and the 2^1S and 2^1P excitations of helium atoms, initially in their ground state, by electron impact. We also compare the scattering of electrons with that of positrons at the same energy.

2. Theory

We expand the total wavefunction of the system in terms of the eigenfunctions $\phi_n(\boldsymbol{r}_i)$ of the unperturbed atom,

$$\Psi(\boldsymbol{r}_i, \boldsymbol{z}) = \sum_{n=0}^{\infty} \phi_n(\boldsymbol{r}_i) a_n(\boldsymbol{b}, z) \exp(\mathrm{i}\boldsymbol{K}_0 \cdot \boldsymbol{z}).$$

Here $\boldsymbol{b}$ is the impact parameter, $\boldsymbol{K}_0$ the velocity of the incident particle, and $\boldsymbol{z} = \boldsymbol{K}_0 t$. Following the procedure described in § 2 of paper II, we obtain coupled integro-differential equations for the amplitudes;

$$\frac{\partial}{\partial z} a_n(b, z) = \frac{1}{\mathrm{i}K_0} \sum_{m=0}^{N} V_{nm}(z) \exp\{\mathrm{i}(\epsilon_n - \epsilon_m) z / K_0\} a_m(b, z) - \frac{1}{K_0^2} \sum_{m=0}^{N} \int_{-\infty}^{z} \mathrm{d}z' K_{nm}(z, z') a_m(b, z')$$

with the boundary conditions $a_n(b, -\infty) = \delta_{0n}$, and the second order potential defined as

$$K_{nm}(z, z') = \sum_{j=N+1}^{\infty} V_{nj}(z') V_{jm}(z') \exp\left(\frac{\mathrm{i}(\epsilon_n - \epsilon_j) z}{K_0} - \frac{\mathrm{i}(\epsilon_m - \epsilon_j) z'}{K_0}\right).$$

This paper deals with the one channel approximation, $N = 0$, in which the elastic amplitude is determined by the equation

$$\frac{\partial}{\partial z}a_0(b, z) = \frac{1}{\mathrm{i}K_0}V_{00}(z)a_0(b, z) - \frac{1}{K_0}\int_{-\infty}^{z} \mathrm{d}z' K_{00}(z, z')a_0(b, z') \tag{1a}$$

where

$$K_{00}(z, z') = \sum_{j=1}^{\infty} V_{0j}(z)V_{j0}(z') \exp\{\mathrm{i}(\epsilon_0 - \epsilon_j)(z - z')/K_0\}. \tag{1b}$$

The 2^1S and 2^1P excitation amplitudes, with distortion, can be computed from these $a_0(b, z)$ by using

$$\frac{\partial}{\partial z}a_n(b, z) = \frac{1}{\mathrm{i}K_0}V_{n0}(z)\exp\left\{\frac{\mathrm{i}(\epsilon_n - \epsilon_0)z}{K_0}\right\}a_0(b, z) + \frac{1}{\mathrm{i}K_0}V_{nn}(z)a_n(b, z). \tag{2}$$

A better approximation for the elastic amplitude is to include the back-couplings from the 2^1S and 2^1P inelastic channels to the ground state, in which case

$$\frac{\partial}{\partial z}a_0(b, z) = \frac{1}{\mathrm{i}K_0}\sum_{m=0,N} V_{0m}(z)\exp\{\mathrm{i}(\epsilon_0 - \epsilon_m)z/K_0\}a_n(b, z) - \frac{1}{K_0^2}\int_{-\infty}^{z} \mathrm{d}z' K_{00}(z, z')a_0(b, z') \tag{3}$$

where $N = 3$ and where the index j in equation (1b) now runs from 4 to ∞. The inelastic amplitudes can similarly be improved by retaining all the direct couplings between the four channels (1^1S, 2^1S and the two independent magnetic substates of 2^1P), leading to the set of equations

$$\frac{\partial}{\partial z}a_n(b, z) = \frac{1}{\mathrm{i}K_0}\sum_{m=0,N} V_{nm}(z)\exp\{\mathrm{i}(\epsilon_n - \epsilon_m)z/K_0\}a_m(b, z) \qquad n \neq 0 \tag{4}$$

The set of coupled equations (3) and (4) are solved simultaneously.

3. Evaluating the cross sections

The matrix elements in equations (1) to (4) are evaluated with the orthogonal helium wavefunctions for the 1^1S, 2^1S and 2^1P states described by Flannery (1970), the measurements of Martin (1960) being used for the 2^1S and 2^1P excitation energies (0·7577 and 0·7799 au). These wavefunctions give rise to the same kind of integrals in the kernel of equation (1) as occurred in paper II when the closure approximation is used.

The coupled integro-differential equations, (1) to (4), are solved numerically by a step-by-step iterative procedure. Then, using Simpson's rule to integrate over the impact parameter b, we arrive at the total excitation cross sections (from paper III),

$$Q(1\mathrm{s}, n) = \frac{2K_n}{K_0}\int_0^{\infty} |a_n(b, \infty) - a_n(b, -\infty)|^2 b\, \mathrm{d}b\ (\pi a_0^2) \tag{5}$$

and the differential cross sections (from Wilets and Wallace 1968),

$$\sigma_{0n}(\theta) = \frac{K_n}{K_0}|f_{0n}(\theta)|^2\ (a_0^2) \tag{6}$$

with

$$f_{0n}(\theta) = (-\mathrm{i})^{m+1}\mu K_0 \int_0^{\infty} \{a_n(b, \infty) - a_n(b, -\infty)\} J_m(2\mu K_0 b \sin \tfrac{1}{2}\theta) b\, \mathrm{d}b$$

where $\mu = 1$ for electron scattering, $a_n(b, -\infty) = \delta_{0n}$ from the boundary conditions and m is the magnetic quantum number of the final state.

The errors arising from the numerical work in this paper are believed to be less than 2%.

4. The effective energy

By replacing $\epsilon_j - \epsilon_0$ in equation (1) with an average energy $\eta = \bar{\epsilon} - \epsilon_0$ as described in paper II, we can remove the infinite sum by using closure. Paper I shows how $\bar{\epsilon}$ can be chosen to ensure that the long range behaviour of the effective potential is

$$\mathrm{Re}(V^{\mathrm{eff}})_{R \xrightarrow{} \infty} -\tfrac{1}{2}\alpha_1 R^{-4} + \mathrm{O}(R^{-6})$$

where α_1 is the dipole polarizability, given by Burke (1968) as 1·39 au. for helium.

In replacing all the levels above the ground state by an effective energy, we find $\eta = 1{\cdot}13$ au. Alternatively, we can use the exact 2^1S and 2^1P energies and average the remaining states, in which case $\eta = 1{\cdot}34$ au, and it is this method which we use here. In paper II there was little difference between the two methods for hydrogen and this is found to be true also for helium. Figure 1 shows the effect of varying η on the elastic cross sections in the single channel approximation of equation (1). Since this is a long range effect, the greatest change is seen at small angles. This agrees qualitatively with Joachain and Mittleman (1971) who found that a variation of η in their imaginary potential affected elastic scattering at large impact parameters, and therefore at small angles.

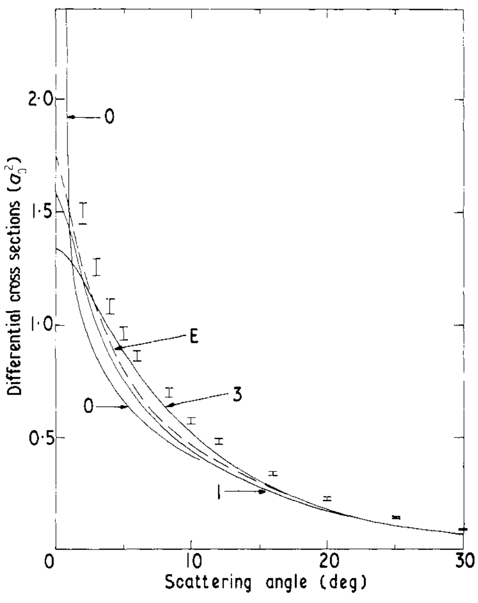

Figure 1. Effect of varying the average energy on the elastic scattering of 500 eV electrons from helium. Curve 0, $\eta = 0{\cdot}0$ au; curve 1, $\eta = 1{\cdot}15$ au; curve 3, $\eta = 3{\cdot}0$ au; curve E, exact energies used for 2^1S and 2^1P states, with $\eta = 1{\cdot}34$ (see text). The experimental data is from Bromberg (1969).

In the forward direction we also agree qualitatively with the second Born approximation of Woollings and McDowell (1972), who found that they had to use a larger effective energy to decrease the real part of the forward scattering amplitude of Holt *et al* (1971b) in order to fit it to the forward dispersion relation results of Bransden and McDowell (1970).

5. Elastic scattering of electrons

Solving equations (3) and (4), with the full static coupling between the 1^1S, 2^1S and 2^1P states and the second order term in the elastic channel, we can use equation (5) to calculate the total cross sections. Our values for elastic scattering are compared in table 1 with the results obtained by omitting the second order term (the four channel static approach of Flannery 1970), the first Born results (B1) of Bell *et al* (1969), the second Born results (B2) of Holt *et al* (1971a), and the experimental results of Vriens *et al* (1968a) and Bromberg (1969).

Table 1. Total cross sections (in πa_0^2) for the elastic scattering of electrons from helium

Energy (eV)	B1	B2	Static	Present results	Experimental†
50	0·714	—	0·557	0·813	—
100	0·412	0·893	0·351	0·415	0·495
200	0·223	0·352	0·200	0·215	0·248
300	0·152	0·211	0·139	0·147	0·170
400	0·115	0·149	0·107	0·107	0·130
500	0·093	0·115	0·087	0·088	0·108‡
1000	0·047	—	0·045	0·045	—

† Vriens *et al* (1968a) renormalized to Chamberlain *et al* (1970).
‡ Bromberg (1969).

At energies below 300 eV inclusion of the second order term increases the cross sections significantly above those evaluated in the static approximation.

In figure 2 we show the effect of various degrees of coupling on the elastic differential cross sections at 300 eV. Keeping the second order term in the elastic channel, we see that the inclusion of the back couplings from the 2^1S and 2^1P channels to the ground state, as in equation (3), only increases the small angle scattering, since the s–p coupling is of long range. However, the inclusion of the 2^1S, 2^1P inter-couplings, as in equation (4), is seen to have no effect in elastic scattering.

Also shown in figure 2 are the results of the eikonal approximation of Joachain and Mittleman (1971), who fixed their effective energy parameter to give the best fit at 5°, the Glauber approximation of Franco (1971), and the second Born approximations of Holt *et al* (1971a) and Woollings and McDowell (1972), who used a much larger value for η.

The essential assumption in the second Born approximation is the replacement of $a_0(b, z')$ by unity in the integral term in equation (3). Comparison with our results shows that this is accurate only for large b and this accounts for the agreement of the second Born cross sections of Holt *et al* (1971a) with our results at small angles, but not at large.

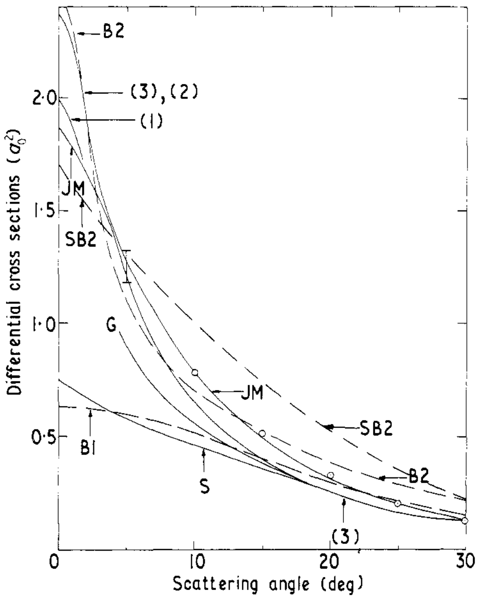

Figure 2. Differential cross sections for the elastic scattering of electrons at 300 eV: comparison of models. Curve (1), Our results with no coupling between the states, but with the second order term in the elastic channel, using equations (1) and (2); curve (2), Our results with the back coupling from the 2^1S and 2^1P channels to the ground state, and the second order term in the elastic channel, using equations (2) and (3); curve (3), Our results with the full static coupling between the 1^1S, 2^1S and 2^1P states and the second order term in the elastic channel, using equations (3) and (4); curve B1, First Born approximation; curve B2, Second Born approximation (Holt *et al* 1971a); curve SB2, Second Born approximation (Woollings and McDowell 1972); curve JM, Eikonal approximation of Joachain and Mittleman (1971), curve G, Glauber approximation of Franco (1970); curve S, Four channel coupling, but without the second order term; I, Chamberlain *et al* (1970); ⊙, Vriens *et al* (1968a), renormalized at 5° to Chamberlain *et al* (1970).

Figure 3 shows that our differential cross sections for the elastic scattering of electrons between 100 and 1000 eV agree well with the experimental data. Less significance can be attached to our results at 50 eV as our model is a high energy approximation and electron exchange, important at low energies, has been ignored. By 1000 eV (see figure 3*c*) our results are becoming quite close to those of the first Born approximation.

6. Forward elastic scattering

In the energy range of figure 4 the differential cross sections evaluated by Bransden and McDowell (1970) using the forward dispersion relations lie well above the present results for forward scattering, though at 1000 eV (see figure 3*c*) we only differ by 7 %. However, our results are consistent with their extrapolations of the experimental data to zero angle above 200 eV. The second Born results of Holt *et al* (1971b) are in better agreement with the data, though this may be due to the choice of the effective energy. Holt *et al* (1971a) used the energy of the 3^1S state, giving $\eta = 0{\cdot}84$ au, compared with our 1·34 au, and as in figure 1 the main effect of this is to slightly increase the forward

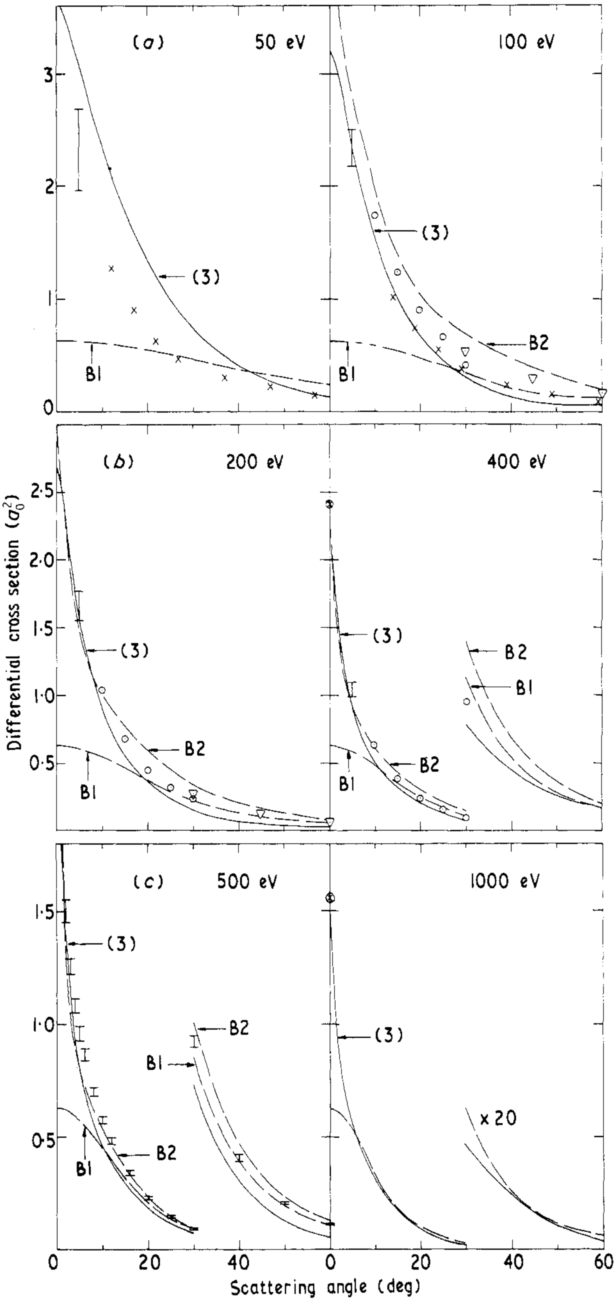

Figure 3. Differential cross sections for the elastic scattering of electrons at (*a*) 50 eV and 100 eV, (*b*) 200 eV and 400 eV, (*c*) 500 eV and 1000 eV.

Curves (3), B1 and B2 are as in figure 2. ○ Vriens *et al* (1968a), renormalized at 5° to Chamberlain *et al* (1970). ▽ Opal and Beaty (1972). × Hughes *et al* (1932). ⊗ Bransden and McDowell (1972), using dispersion relations. I Bromberg (1969) at 500 eV, otherwise Chamberlain *et al* (1970).

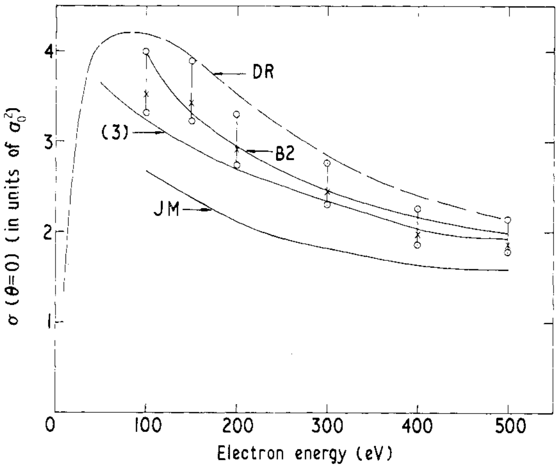

Figure 4. Elastic differential cross sections in the forward direction. Curves (3), B2 and JM are as in figure 2. Curve DR. Dispersion relation results of Bransden and McDowell (1970). Extrapolations of the data to zero angle by Bransden and McDowell (1970).

scattering. Notice that the eikonal approximation of Joachain and Mittleman (1971) underestimates the scattering in the forward direction.

Our values for the real part of the forward elastic scattering amplitude for 50, 100, 200, 300, 400, 500 and 1000 eV are 1·48, 1·39, 1·28, 1·22, 1·15, 1·13 and 1·02 au. These are from 30%–10% smaller than the dispersion relation (DR) results of Bransden and McDowell (1970), but in better agreement with the DR results than either the lower values given by the eikonal approximation of Joachain and Mittleman (1971) and the Padé approximation of Garibotti and Massaro (1971), or the very high values given by the second Born approximation of Holt *et al* (1971b).

7. The 2^1S excitation of helium by electrons

Our total cross sections, evaluated with the full static coupling between the 1^1S, 2^1S and 2^1P states and the second order term in the elastic channel, are shown in table 2

Table 2. Total cross sections (in units of $10^{-3}\pi a_0^2$) for the 2^1S excitation of helium by electrons

Energy (eV)	B1	SB2	Static	Present results	Experimental	
50	38·1	—	31·0	22·5	(18±9)§	—
100	22·5	—	18·2	15·4	—	21·0‡
200	11·8	10·4	10·2	9·26	6·7†	11·2
300	7·97	7·28	7·07	6·64	5·3	7·6
400	6·03	5·64	5·43	5·20	4·7	5·7
500	4·85	4·57	4·40	4·24	—	—
1000	2·45	—	2·27	2·23	—	—

† Vriens *et al* (1968b) renormalized to Chamberlain *et al* (1970).
‡ Lassettre (1965).
§ Rice *et al* (1972) at 55·5 eV.

for the 2^1S excitation. These are compared with the first Born cross sections (B1) of Bell *et al* (1969), the second Born results (SB2) of Woollings and McDowell (1972), and the results using the four channel static approach of Flannery (1970). Our results are in good agreement with the experimental data shown in table 2, particularly with that of Vriens *et al* (1968b). Notice that at all energies our total cross sections are lowered by the inclusion of the second order term.

Figure 5 shows the effects of various approximations on the differential cross sections for the 2^1S excitation by 300 eV electrons. The inclusion of the second order term has little effect on the static approximation, though there is a marked discrepancy when the inter-coupling between the 2^1S and 2^1P states is omitted. This shows the importance of the 2^1S–2^1P coupling in the 2^1S excitation angular distributions, and by ignoring this coupling the Born results are too low in the forward direction.

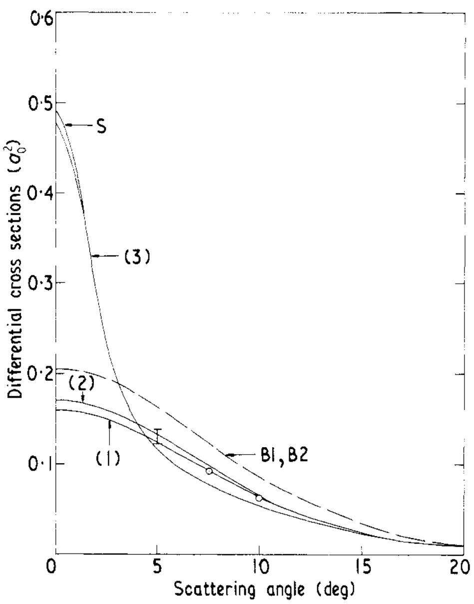

Figure 5. Differential cross sections for the 2^1S excitation of helium by 300 eV electrons. Comparison of models.

Curves (1), (2), (3), S, B1 and B2 are as in figure 2. I Chamberlain *et al* (1970); ⊙ Vriens *et al* (1968b), renormalized at 5° to Chamberlain *et al* (1970).

Figure 6 shows the 2^1S excitation differential cross sections for a range of energies, significant improvement being made over the Born results. In figure 6*c* we show the simplified second Born results of Woollings and McDowell (1972). Although we saw in figure 2 that their elastic differential cross sections were too large, they improved upon the 2^1S and 2^1P excitation results of Holt *et al*, who found nearly the same angular distribution as that calculated from the first Born approximation.

In all our graphs the first Born differential cross sections for the 2^1S and 2^1P excitations were deduced from the generalized oscillator strengths calculated by Kim and Inokuti (1968).

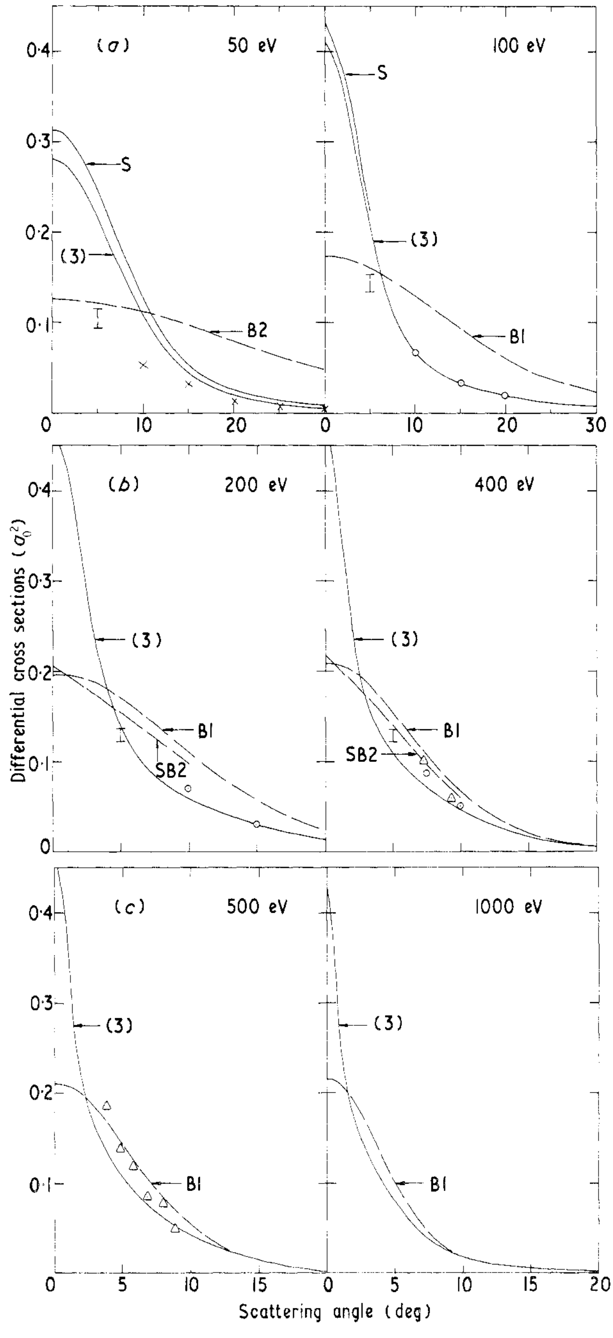

Figure 6. Differential cross sections for the 2^1S excitation of helium by electrons at (*a*) 50 eV and 100 eV, (*b*) 200 eV and 400 eV, (*c*) 500 eV and 1000 eV.

Curves (3), S, B1 and SB2 are as in figure 2. ⊙ Vriens *et al* (1968b), renormalized at 5° to Chamberlain *et al* (1970); △ Lassettre *et al* (1964) at 417 eV and 511 eV; I Chamberlain *et al* (1970); × Rice *et al* (1972) at 55·5 eV.

8. The 2^1P excitation of helium by electrons

Table 3 shows the results with the full static coupling between the 1^1S, 2^1S and 2^1P states, and the second order term in the elastic channel. This is compared with the results using the four channel static approach of Flannery (1970) and the first Born results of Bell *et al* (1969). Only below 100 eV does the effect of the second order term become noticeable.

Table 3. Total cross sections in units of πa_0^2 for the 2^1P excitation of helium by electrons

Energy (eV)	Born	Static	Present results
50	0·169	0·232	0·215
100	0·148	0·161	0·155
200	0·107	0·107	0·105
300	0·0841	0·0830	0·0822
400	0·0699	0·0685	0·0681
500	0·0602	0·0584	0·0581
1000	0·0367	0·0362	0·0362

A large amount of data has recently become available on the total excitation cross sections for the 2^1P state (see Donaldson *et al* 1972). This is displayed in figure 7 together with our total cross sections. Although there appears to be a maximum in the experimental data between 60 eV (Moustafa Moussa *et al* 1969) and 85 eV (Donaldson *et al* 1972), our results show a steep rise below 100 eV and further investigation is required in this energy region.

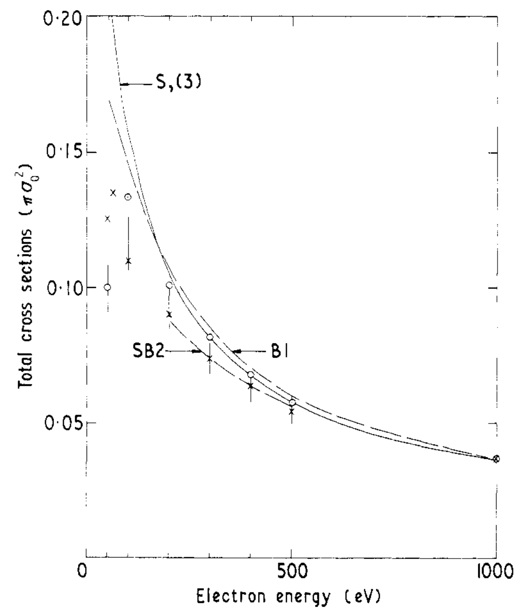

Figure 7. Total cross sections for the $1^1S \rightarrow 2^1P$ excitation of helium by electron impact. Curves (3), S, B1, B2 and SB2 are as in figure 2. ○ Van Eck and de Jongh (1970); × Moustaffa Moussa *et al* (1969); | Donaldson *et al* (1972).

Figure 8 shows the effect of various approximations on the differential cross sections for the 2^1P excitation by 300 eV electrons, where it is shown that the inclusion of back-coupling to the ground state as in equation (3) has a small effect on the angular distribution. The strong 1^1S–2^1P coupling completely swamps any effect similar to that observed in the 2^1S excitation, where omission of the 2^1S–2^1P coupling altered the results considerably.

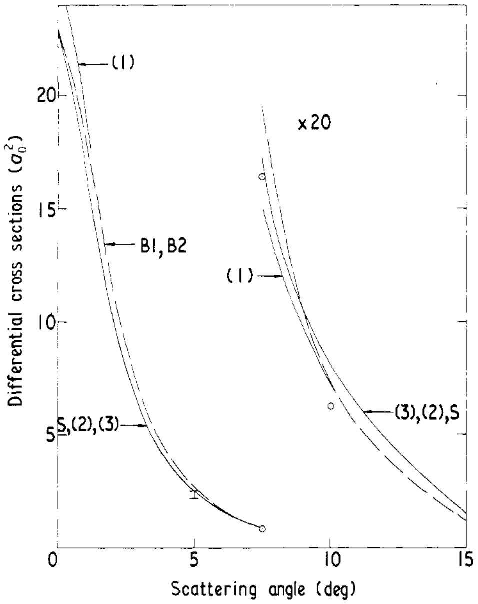

Figure 8. Differential cross section for the 2^1P excitation of helium by 300 eV electrons: comparison of models. Curves (1), (2), (3), S, B1 and B2 are as in figure 2. Ɪ Chamberlain *et al* (1970); ○ Vriens *et al* (1968b), renormalized at 5° to Chamberlain *et al* (1970).

Figure 9 shows the 2^1P excitation differential cross sections for a range of energies. Again significant improvement is made over the Born results.

Flannery (1970) noticed that the effect of the four-channel couplings is to reduce the percentage polarization of emitted radiation, P_e, as compared to the first Born approximation. Using his equation (23), derived by Percival and Seaton (1958), we calculate P_e with our results and find that, as shown in table 4, the addition of the second order term causes a slight increase over the results using the static approach of Flannery (1970).

9. The scattering of positrons from helium

By reversing the sign of the potential we can compare the scattering of electrons with that of positrons in the same approximation. At a fixed energy, the cross sections given by the first Born and the static approximations are unaffected by the change in sign, but figure 10 shows that the inclusion of the second order term at 300 eV causes a significant difference in the angular distributions, particularly for elastic scattering where the forward peak is almost absent for positrons. We find the total cross sections for 300 eV positrons to be 0·133, 0·0090 and 0·0829 (πa_0^2) for the 1^1S, 2^1S and 2^1P excitations of

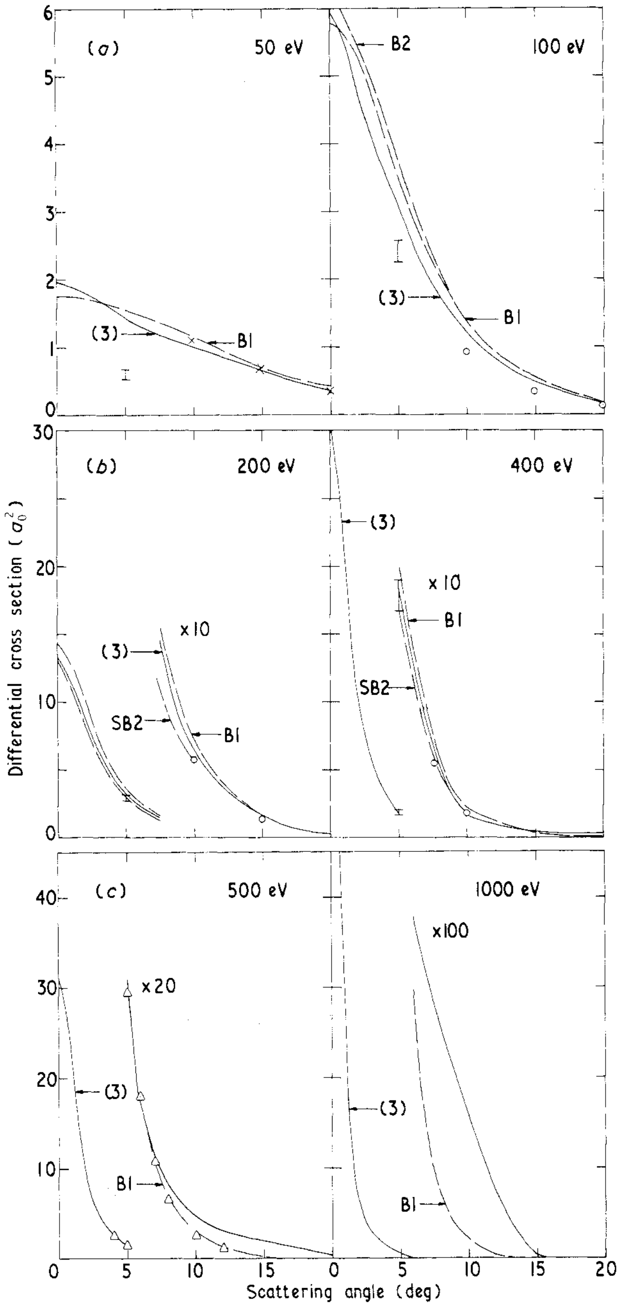

Figure 9. Differential cross sections for the 2^1P excitation of helium by electrons at (*a*) 50 eV and 100 eV, (*b*) 200 eV and 400 eV, (*c*) 500 eV and 1000 eV. Curves (3), B1 and SB2 are as in figure 2. ⊙ Vriens *et al* (1968b), renormalized at 5° to Chamberlain *et al* (1970); △ Lassettre *et al* (1964) at 511 eV; I Chamberlain *et al* (1970); × Truhlar *et al* (1970) at 55·5 eV as renormalized by Rice *et al* (1972).

Table 4. Percentage polarization, P_e, of radiation following excitation of He(2^1P) by electrons.

Energy (eV)	Static	Present results
50	3·14	3·59
100	−0·15	−0·03
200	−3·10	−3·01
300	−4·31	−4·24
400	−5·80	−5·35
500	−6·51	−6·45
1000	−7·63	−7·63

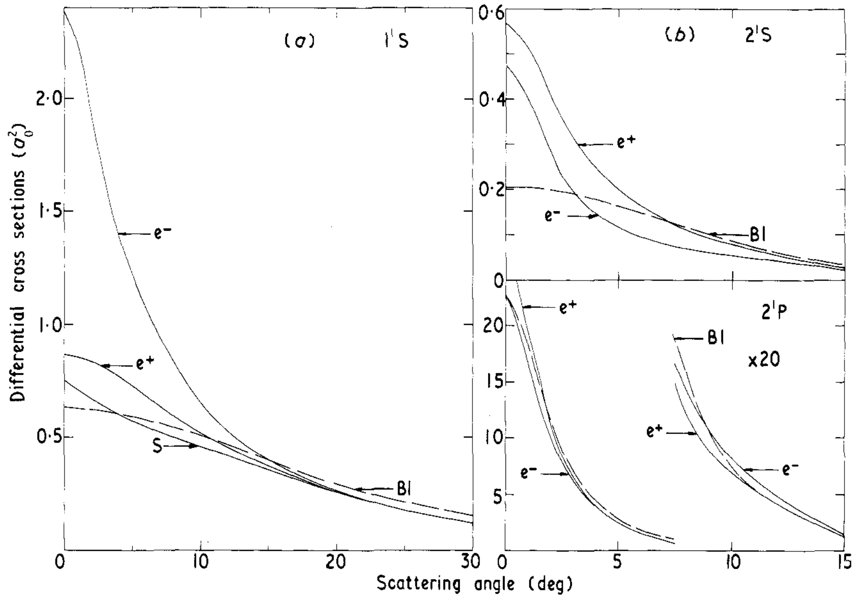

Figure 10. Comparison of electron and positron scattering from helium at 300 eV, differential cross sections for (*a*) elastic scattering, (*b*) the 2^1S and 2^1P excitations.

Curves (e^-) and (e^+). Our results for e^- and e^+ respectively, using equations (3) and (4). Curves S and B1 are as in figure 2.

helium. Comparing these with the values quoted for electrons in tables 1, 2 and 3, we find a reduction in elastic scattering and an increase in the 2^1S and 2^1P excitations of helium by positron impact.

10. Conclusion

The results are significantly better than those obtained without allowance for the channels not explicitly included, and, as was shown in paper III for hydrogen, our method lends itself to systematic improvement by the addition of further first and second order couplings.

For elastic scattering, the eikonal approximation of Joachain and Mittleman (1971) is good at angles greater than about 2°, but our results give better agreement in the forward direction with the dispersion relation results and the extrapolation of data to zero angle by Bransden and McDowell (1970).

Our results also compare well with the second Born approximations, and we note that although Woollings and McDowell (1972) found their method gave a better description for the 2^1S and 2^1P excitations than that given by Holt *et al* (1971a), it overestimates the elastic scattering.

Finally, we do not expect our approximations to be valid at low energies. Work is at present in progress in the region 20–100 eV without the impact parameter assumption and making allowance for exchange.

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