J. Phys. B: Atom. Molec. Phys., Vol. 8, No. 17, 1975. Printed in Great Britain. © 1975

High energy elastic scattering of electrons from the 2^1S and 2^3S states of helium

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Received 3 September 1974, in final form 14 July 1975

Abstract. Differential and total elastic cross sections are given in the first Born approximation for electrons incident on the ground and metastable (2^1S and 2^3S) states of helium. Unrestricted Hartree–Fock wavefunctions have been employed and for the ground state the resultant differential cross section is compared with those obtained using unrestricted Hartree–Fock and many-parameter wavefunctions. For the metastable states the differential cross section is very strongly peaked in the forward direction and the total cross sections are an order of magnitude larger than that for the ground state.

1. Introduction

Excited states of atoms are of increasing interest in astrophysics and plasma physics but at present there are little data on their properties. Long-lived metastable states are of particular importance and experiments with atomic beams including such particles are now being carried out. For metastable helium a number of calculations of excitation or ionization cross sections have been published (Kim and Inokuti 1969 and references therein, Briggs and Kim 1971) but elastic scattering data is only available at quite low energies (eg Sklarew and Callaway 1968, Robinson 1969) apart from one calculation by Bhattacharyya (1961) at 700 eV. Neynaber *et al* (1964) have measured the total cross section for 2^3S helium at low energies. In the present work the differential and total elastic scattering cross sections for high energy electrons incident on 2^1S and 2^3S helium have been calculated using the first Born approximation. The matrix elements obtained have also been used by Buckley and Walters (1975) in second Born calculations on the electron excitation of the ground state.

2. Theory

For electrons of incident energy $E = \frac{1}{2}k^2$ au†, with initial momentum $k\boldsymbol{n}_i$ and final momentum $k\boldsymbol{n}_f$, $\boldsymbol{n}_i$ and $\boldsymbol{n}_f$ being unit vectors, the differential elastic cross section for helium in the first Born approximation may be expressed as

$$I(K) = \frac{4}{K^4}|\epsilon(K)|^2 \tag{1}$$

† Atomic units are used throughout this paper, except in § 3 where total cross sections are given in cm^2 and the corresponding incident electron energies in eV.

where $\boldsymbol{K} = k(\boldsymbol{n}_i - \boldsymbol{n}_f)$ is the change of momentum in the collision and is related to the scattering angle θ by

$$\sin\tfrac{1}{2}\theta = K/(2k).$$

The elastic matrix element $\epsilon(K)$ is

$$\epsilon(K) = \iint \Psi(\boldsymbol{r}_1, \boldsymbol{r}_2)[\exp(\mathrm{i}\boldsymbol{K}\,.\,\boldsymbol{r}_1) + \exp(\mathrm{i}\boldsymbol{K}\,.\,\boldsymbol{r}_2) - 2]\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2)\,\mathrm{d}\boldsymbol{r}_1\,\mathrm{d}\boldsymbol{r}_2 \qquad (2)$$

where $\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is the wavefunction for the atomic state. The elastic scattering cross section is then given by

$$Q(E) = \frac{\pi}{E}\int_0^{2k} KI(K)\,\mathrm{d}K. \qquad (3)$$

The differential cross section $I(K)$ and the total cross section $Q(E)$ have both been evaluated for the two metastable states. In addition, the ground-state cross sections have also been calculated to show the different magnitudes of the cross sections and to provide a guide to the accuracy of the results.

The present work involves two approximations: one caused by using the first Born approximation and the second by employing approximate wavefunctions to evaluate the Born matrix elements (2). The present wavefunctions are numerical unrestricted Hartree–Fock (UHF) functions in which the inner orbital is frozen (see Bell *et al* 1968). Such wavefunctions generally give a better representation of excited states than of the ground state. In the present case the 2^1S and 2^3S energies are $-2{\cdot}1434$ and $-2{\cdot}1742$ respectively which may be compared with the accurate non-relativistic energies of $-2{\cdot}1460$ for 2^1S and $-2{\cdot}1752$ for 2^3S (Pekeris 1962). The corresponding UHF ground-state energy is $-2{\cdot}873$ compared to the accurate value of $-2{\cdot}904$.

3. Results and discussion

3.1. Differential elastic cross sections

Table 1 gives the differential cross sections $I(K)$ for the metastable states obtained from equation (1) and calculated with the unrestricted Hartree–Fock wavefunctions. For the ground state the results of Kennedy (1968), who employed a 52-parameter Hylleraas-type wavefunction, are compared with the present UHF values. The cross sections for the excited states are much larger for small momentum transfers K than that for the ground state, being strongly peaked in the forward direction. At higher values of K the cross sections approach one another, those for the 2^1S and 2^3S states being within 1 % of each other above $K = 3$ and within 10 % of the 1^1S value above $K = 4$.

An indication of the accuracy of the unrestricted Hartree–Fock approximation is given by comparing the present 1^1S results with those of Kennedy (1968). The UHF value for $I(0)$ is 7 % higher than that for the more accurate 52-parameter calculation, but above $K = 5$ the agreement is better than 1 %. Kolos and Pecul (1961) and Kim and Inokuti (1968) have also considered the accuracy of Hartree–Fock wavefunctions for evaluating the helium 1^1S elastic cross section. With a closed-shell Hartree–Fock wavefunction Kim and Inokuti obtained a value for $I(0)$ within 1·5 % of the accurate

Table 1. First Born elastic differential cross sections $I(K)$ (in au sr^{-1}) for electron collisions with helium and asymptotic coefficients in expansion (4).

Atomic state	2^3S	2^1S	1^1S	1^1S
	Unrestricted Hartree–Fock wavefunctions			52-parameter wavefunction (Kennedy 1968)
Change in momentum K (au)	Elastic differential cross section, $I(K)$			
0·0	5·942^{1}†	1·229^{2}	6·765^{-1}	6·331^{-1}
0·1	5·724^{1}	1·166^{2}	6·741^{-1}	6·310^{-1}
0·2	5·126^{1}	9·994^{1}	6·672^{-1}	6·247^{-1}
0·3	4·296^{1}	7·830^{1}	6·559^{-1}	
0·4	3·403^{1}	5·698^{1}	6·406^{-1}	6·006^{-1}
0·5	2·578^{1}	3·929^{1}	6·216^{-1}	
0·6	1·892^{1}	2·620^{1}	5·994^{-1}	5·633^{-1}
0·8	9·714	1·135^{1}	5·480^{-1}	5·165^{-1}
1·0	4·999	5·184	4·908^{-1}	4·642^{-1}
1·4	1·577	1·497	3·748^{-1}	
1·8	6·566^{-1}	6·272^{-1}	2·736^{-1}	
2·2	3·357^{-1}	3·270^{-1}	1·949^{-1}	
2·6	1·951^{-1}	1·926^{-1}	1·377^{-1}	
3·0	1·228^{-1}	1·221^{-1}	9·752^{-2}	
4·0	4·733^{-2}	4·733^{-2}	4·301^{-2}	
5·0	2·171^{-2}	2·172^{-2}	2·070^{-2}	2·052^{-2}
6·0	1·116^{-2}	1·117^{-2}	1·086^{-2}	
Asymptotic coefficients				
S	−1·2040	−1·1798	−1·5331	
T	−7·579^{1}	−7·777^{1}	−9·713^{1}	

† Superscript denotes the power of 10 by which the number is to be multiplied.

many-parameter value, with the agreement improving at higher values of K. This better agreement with accurate values can only be because they employ a restricted (or closed-shell) wavefunction while the present 1^1S representation is an unrestricted (or open-shell) approximation. This suggests that where the electrons in an atom form closed shells the restricted form of the Hartree–Fock approximation gives better results for the elastic cross section than does the UHF approximation. For helium excited states the unrestricted form of the Hartree–Fock approximation must be employed. The values quoted for the 2^1S and 2^3S elastic cross sections should be at least as accurate as the present 1^1S results.

Further information on the accuracy of the metastable cross sections is provided by the forward scattering limit. In the first Born approximation this limit $I(0)$ is given by the matrix element $\frac{4}{9}|\langle\Psi|r_1^2|\Psi\rangle|^2$ which may be evaluated accurately with many-parameter wavefunctions. Using the very accurate results of Pekeris (1962), the forward scattering limit was calculated to be 0·6331, 115·0 and 58·4 for the elastic scattering of the 1^1S, 2^1S and 2^3S states respectively. By comparison, the corresponding UHF values are 7 %, 7 % and 2 % larger. It seems likely that the present UHF values of $I(K)$ for the metastable states will be more accurate at higher values of K, just as for the ground state.

For large momentum transfers K, values of the differential cross section may be fitted to

$$I(K) = \frac{16}{K^4}\left(1+\frac{S}{K^2}+\frac{T}{K^4}\right) \tag{4}$$

where S and T are constants, dependent on the atomic state. In the present case S and T, given in table 1, were determined by fitting to calculated UHF values of $I(K)$ for K between 6·0 and 10·0. Then the function (4) represents $I(K)$ to better than 1 % for $K \geqslant 6$.

The differential elastic cross section for the 2^1S state has also been calculated in the first Born approximation by Bhattacharyya (1961) using hydrogenic wavefunctions. While her tabulated values of the cross section are for 700 eV electrons, using her published formula it is possible to recalculate $I(K)$ directly as a function of K. With effective charges $Z = 2$ and $Z = 1$ for inner and outer electrons respectively, $I(K)$ diverges at $K = 0$ but agrees with the present UHF values to better than 4 % for $K \geqslant 1·0$.

As is well known (Mott and Massey 1965) the first Born approximation fails at both small and large scattering angles, especially if the incident electron energy is not sufficiently high. For the ground state comparison between experiment and various theoretical calculations at intermediate energies has been carried out by Byron and Joachain (1973a, b). For energies between 100 eV and 400 eV their eikonal-Born series calculations are in reasonable agreement with the experimental data of Vriens *et al* (1968), as renormalized by Chamberlain *et al* (1970), and with Crooks and Rudd (1972). At 500 eV their calculations are in excellent agreement with the very accurate experiments of Bromberg (1969). Between these energies of 100 eV and 500 eV, the Born approximation agrees quite well with experiment if $K \geqslant 2·0$, corresponding to scattering angles of 43° at 100 eV and 19° for 500 eV electrons. For large scattering angles the Born approximation again falls below the experimental values. These observations are confirmed by the recent experiments of Sethuraman *et al* (1974) and McConkey and Preston (1975). Since no experimental results have been published on the differential elastic cross sections for metastable helium it is not yet possible to decide for which angles and over what energy range the first Born approximation applies.

3.2. Total elastic cross sections

Table 2 presents the first Born cross sections (equation (3)) for the elastic scattering of electrons with helium atoms in the ground and metastable states, calculated from the unrestricted Hartree–Fock matrix elements $I(K)$. The cross sections for the two metastable states are considerably larger than that for the ground state, the 2^1S cross section being a factor of eleven larger and the 2^3S a factor of eight larger than the 1^1S cross section at 100 eV, with these ratios decreasing slightly at higher energies. Starostin (1967) has shown that at high energies in the first Born approximation the cross sections for excited states increase as n^4 when n is very large, where n is the principal quantum number of the outer electron. For the metastable states the increases in the cross section over the ground state are rather smaller at high energies than this factor would indicate but, considering that n only changes from 1 to 2, the agreement is quite good.

Also shown in table 2 are the first Born elastic scattering cross sections of Bell *et al* (1969) obtained with a 52-parameter wavefunction for the ground state. Above 100 eV, the present UHF values are up to 6 % greater than these more accurate results, compared to the case for the differential cross section where the largest difference was 7 % in the forward direction. It seems reasonable to expect that in a similar manner the metastable

Table 2. First Born total elastic cross sections $Q(E)$ (in 10^{-17} cm^2) for electron collisions with helium and asymptotic coefficients in expansion (5).

Atomic state	2^3S	2^1S	1^1S	1^1S
	Unrestricted Hartree–Fock wavefunctions			52-parameter wavefunction (Bell *et al* 1969)
Incident electron energy, E(eV)	Elastic cross section, $Q(E)$			
0	2·091^{3}	4·323^{3}	2·380^{1}	2·228^{1}
5	4·838^{2}	7·312^{2}	1·834^{1}	
10	2·677^{2}	3·902^{2}	1·537^{1}	
20	1·415^{2}	2·025^{2}	1·145^{1}	
30	9·680^{1}	1·644^{2}	9·417	8·869
50	5·945^{1}	8·383^{1}	6·837	6·282
100	3·012^{1}	4·231^{1}	3·795	3·626
150	2·017^{1}	2·829^{1}	2·613	2·544
200	1·518^{1}	2·127^{1}	2·013	1·958
300	1·017^{1}	1·423^{1}	1·389	1·340
Asymptotic coefficients				
A	3·0709^{3}	4·2895^{3}	4·3724^{2}	
B	−6·5133^{3}	−6·5133^{3}	−6·5133^{3}	
C	1·3336^{4}	1·3068^{4}	1·6982^{4}	
D	1·904^{6}	1·953^{6}	2·440^{6}	

cross sections are above the exact Born values by less than 7 % for 2^1S and 2 % for 2^3S, these being the errors in the forward differential cross sections caused by the approximate wavefunctions.

For large incident electron energies E (in eV) the elastic cross section Q(in 10^{-17} cm^2) may be represented by

$$Q(E) = \frac{A}{E} + \frac{B}{E^2} + \frac{C}{E^3} + \frac{D}{E^4} \tag{5}$$

where A, B, C and D are constants. A is the differential cross section function $KI(K)$, integrated over all values of K while B, C and D are derived by integration of the three-term asymptotic expansion (4) for $I(K)$, B being a constant independent of the atomic state. With the resultant values for the constants, shown in table 2, equation (5) represents the ground-state cross section to better than 1 % for E greater than 100 eV. The UHF value for A is 6 % higher than the 52-parameter value of Bell *et al* (1969) obtained by fitting an asymptotic expansion directly to their calculated cross sections. For the metastable states the cross section is given by equation (5) to better than 1 % if E is between 30 and 100 eV and within 0·1 % if E is greater than 100 eV. Above 300 eV equation (5) may be used to generate without significant error further values of the cross sections.

By comparing with other theoretical and experimental values the accuracy of the present 1^1S-total elastic cross section results may be evaluated. Unfortunately, Byron and Joachain (1973a, b) have not published total elastic cross sections from their differential results. Comparison with the extended polarization calculation of LaBahn and Callaway (1969) shows that the first Born values are 40% lower at 100 eV and 15% lower at 400 eV. The experimental cross sections indicate a similar accuracy. The present values are 46% lower at 100 eV and 20% lower at 300 eV than the data of Vriens *et al* (1968) and 14% lower than that of Bromberg (1969) at 500 eV. These observations show that in the intermediate energy region around 100 eV the first Born approximation can only give results accurate to within an order of magnitude but at higher energies above 400 eV it becomes increasingly reliable.

For the metastable states no other high energy calculation of the total elastic cross sections appears to have been carried out. At energies of a few eV, a number of calculations have been performed (eg Sklarew and Callaway 1967, Robinson 1969) but these energies are too low to compare their results with the high energy Born approximation. However they do show that at low energies the $2^{1,3}$S elastic cross sections are very much larger than the 1^1S cross section. This relationship appears to hold also in the high energy region for, as table 2 indicates, the $2^{1,3}$S cross sections are an order of magnitude larger than that for the ground state.

In considering the accuracy of the present results for the metastable states it should be noted that the ionization potential of the outer electron in these states is a factor of 5–6 lower than that for the ground state. The Born approximation is more accurate when the incident electron energy is much greater than the ionization potential, indicating that it should be reliable to much lower energies for the metastable states than for the ground state. In the latter case the Born approximation is within 14% of accurate experimental data at 500 eV so from the above considerations, the accuracy of the metastable cross sections should be better than 14% for energies considerably less than 500 eV.

Acknowledgments

I should like to thank the Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast for assistance with this research and in particular Drs A E Kingston and K L Bell for their advice and guidance given during this work.

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