J. Phys. B: Atom. Molec. Phys., Vol. 6, November 1973. Printed in Great Britain. © 1973

Double excitation of helium by electron impact

E S Gillespie†

Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast

Received 10 January 1973, in revised form 23 July 1973

Abstract. Cross sections for the electronic excitation of the $(ns, mp)\,^1P$ states (for $n, m = 2, 3, 4$) from the ground state are calculated using the Born approximation and multi-parameter Hylleraas-type wavefunctions. The influence of the interelectron coordinate r_{12} is discussed.

1. Introduction

Calculations of double excitation cross sections for ^1P states of helium have been carried out by Massey and Mohr (1935). They take the Eckhart function, Eckhart (1930), for the ground state of atomic helium, while for the doubly excited states they pick the approximate wavefunctions of Vinti (1932). From McDowell and Coleman (1970) we note that calculations of multiple excitation processes in helium will, if the first Born approximation is used, be valid only for correlated wavefunctions describing the ground state. In this paper cross sections for electronic impact excitation of helium to one of its doubly excited configurations $(2s, np)\,^1P$ and $(ns, 2p)\,^1P$ (for $n = 2, 3, 4$) are calculated using the more accurate multi-parameter Hylleraas-type wavefunctions for the ground state. The interaction of the excited states with the continuum is ignored as the cross sections are intended as a guide to the corresponding cross sections for excitation to the states $(2s, kp)\,^1P$ and $(2p, ks)\,^1P$. Also for the doubly excited atoms which are of interest as reaction initiators in radiation chemistry, electron exchange has been neglected on account of the relatively large energy of the incident electrons.

2. Theory

The wavefunction describing the final state of the system is approximated by a linear symmetrized combination of terms involving the wavefunctions of the excited states under consideration.

$$u(\boldsymbol{r}_1, \boldsymbol{r}_2) = N(\phi_1(\boldsymbol{r}_1)\phi_2(\boldsymbol{r}_2) + \phi_1(\boldsymbol{r}_2)\phi_2(\boldsymbol{r}_1))\chi(1, 2) \tag{1}$$

where the functions $\phi(\boldsymbol{r})$ represent the spatial parts of the hydrogenic states, each subscript standing for an entire set of quantum numbers, $\chi^-(1, 2)$ represents the singlet spin state and N is a normalization constant. Thus for a ^1P state (1) becomes

$$u(\boldsymbol{r}_1, \boldsymbol{r}_2) = 2^{-1/2}(\phi_{ns}(Z, \boldsymbol{r}_1)\phi_{n'p}(Z^1, \boldsymbol{r}_2) + \phi_{ns}(Z, \boldsymbol{r}_2)\phi_{n'p}(Z^1, \boldsymbol{r}_1)) \tag{2}$$

where Z and Z^1 are screened nuclear values.

† Now at: The School of Physical Science, Ulster College, The Northern Ireland Polytechnic.

From the symmetry of the atomic electrons, the scattering amplitude is

$$f(\boldsymbol{\kappa}) = -\frac{4}{\kappa^2}\int \Psi_f^*(\boldsymbol{r}_1, \boldsymbol{r}_2)\exp(\mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{r}_1)\Psi_i(\boldsymbol{r}_1, \boldsymbol{r}_2)\,\mathrm{d}\boldsymbol{r}_1\,\mathrm{d}\boldsymbol{r}_2 \tag{3}$$

where $\Psi_f(\boldsymbol{r}_1, \boldsymbol{r}_2)$ and $\Psi_i(\boldsymbol{r}_1, \boldsymbol{r}_2)$ are the final and initial state wavefunctions. As one of the main objects is to examine the influence of the interelectron repulsion term on the cross sections, three-, six- and ten-parameter Hylleraas-type wavefunctions are taken to represent the ground state, Hylleraas (1929, 1930), Stewart *et al* (1963) and Chandrasekhar *et al* (1953).

3. Results and discussion

To ensure convergence of the cross sections it is necessary to include ten parameters in the ground state wavefunction of helium, Chandrasekhar *et al* (1953). The convergence is illustrated in table 1 for the (2s2p) ^{1}P state with $Z = Z^1 = 2{\cdot}00$.

Table 1. Electron cross sections $Q(10^{-4}\pi a_0^2)$ for excitation of (2s2p) ^{1}P state using multi-parameter functions

Parameter number \ Energy (Ryd)	8	10	15	20	30
3	9·20	8·96	7·92	6·82	5·52
6	11·8	12·1	11·3	10·2	8·40
10	12·9	13·0	11·9	10·5	8·53

Preliminary calculations have shown that if the above multi-parameter functions represent the ground state, the cross sections are much more sensitive to the choice of Z than on Z^1 and in all cases the nuclear charge has been assigned to the 2s state. The value $Z^1 = 1{\cdot}58$ was chosen so that we could compare the cross sections with those in which an Eckhart wavefunction described the initial state.

However it is obvious that a value of Z^1 should be chosen with some conviction and this was done by calculating the oscillator strength for (2s2p) ^{1}P state and picking the value of Z^1 which gave the experimental value. This value was found to be $Z^1 = 1{\cdot}80$. From table 2 we note the large variation in cross section when the value of Z^1 changes from 1·58 to 1·80.

Table 2. Electron cross sections $Q(10^{-4}\pi a_0^2)$ for excitation of (2s2p) ^{1}P state using 1 10-parameter function

Z^1 \ Energy (Ryd)	8	10	15	20	30
1·58	6·42	6·52	5·99	5·34	4·35
1·80	9·55	9·63	8·83	7·87	6·39

This variation is also observed when one uses either the Hartree–Fock function of Green *et al* (1954) or the closed shell function of Eckhart (1930) to describe the ground state of helium and it stresses the need for a reliable value of Z^1 or more accurately improved wavefunctions for the doubly excited states. Also it will be noted that with $Z^1 = 1{\cdot}80$ the cross sections obtained are comparable to those of Massey and Mohr (1935). Consideration of this last point leads one to the conclusion that supplementary experimental work on the electronic excitation of the (2s 2p) ^{1}P state of helium would be a decided advantage in lending credibility to the theoretical cross sections.

For the states (2s, np) ^{1}P and (ns, 2p) ^{1}P (for $n = 3, 4$) the values of Z^1 and Z respectively do not offer the screening problem as that mentioned for the (2s2p) ^{1}P state and the selected values are those chosen by Massey and Mohr (1935). Also on account of the smaller overlap, a 6-parameter function only is necessary to ascertain convergence (table 3).

Table 3. Electron cross sections $Q(10^{-5}\pi a_0^2)$ for excitation of (ns, mp) ^{1}P state

n, m \ Energy (Ryd)	8	10	15	20	30
2, 3	3·16	3·27	3·05	2·74	2·24
2, 4	1·32	1·38	1·30	1·17	0·96
3, 2	50·6	63·1	74·2	74·7	69·1
4, 2	31·8	39·4	45·9	46·0	42·4

From table 3 we note that the results are at least in qualitative agreement. Thus for high energies of the incident electrons, one would expect that for a given Z and Z^1, the cross sections would vary as m^{-3}. To a large extent this is so as may be seen by comparing the cross sections for '30 Ryd' electrons when $Z^1 = 1{\cdot}00$.

4. Conclusion

Referring to table 1 we note the decrease in significance of the interelectron term as the energy of the incident electrons is increased. This is what would be expected on physical grounds as one would deem the interelectron energy small compared to twenty or thirty rydbergs. However even for high energies of the incident electrons there is still great disparity in cross sections for the helium ground state being described by a Hartree–Fock function and a multi-parameter Hylleraas-type function, Gillespie (1970). In view of this we therefore conclude that although the cross sections are at least in qualitative agreement with theory, it would be desirable to have an experimental indication of the cross sections.

Acknowledgments

I would like to thank Professor B L Moiseiwitsch for suggesting the problem of double excitation and for his valuable guidance in the preliminary stages of the investigation.

References

Chandrasekhar S, Herzberg G and Elbert D 1953 *Phys. Rev.* **91** 1172–3
Eckhart C 1930 *Phys. Rev.* **36** 878–92
Gillespie E S 1970 *Thesis* The Queen's University of Belfast
Green L C, Mulder M M, Lewis M N and Woll J W 1954 *Phys. Rev.* **93** 757–61
Hylleraas E A 1929 *Z. Phys.* **54** 347–66
—— 1930 *Z. Phys.* **60** 624–30
Massey H S W and Mohr C B O 1935 *Proc. Camb. Phil. Soc.* **31** 604–8
McDowell M R C and Coleman J P 1970 *Introduction to the Theory of Ion–Atom Collisions* (London: North-Holland) pp 307–72
Stewart A L and Webb T G 1963 *Proc. Phys. Soc.* **82** 532–6
Vinti J P 1932 *Phys. Rev.* **42** 632–40