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Exchange excitation of helium by electron impact

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Abstract. Cross sections for the excitation of the 2^3P and 3^3P states of helium from the ground state by electron impact are calculated using Ochkur approximation. Results are compared with various theoretical cross sections and experimental data.

1. Introduction

Although a great deal of experimental and theoretical effort has gone into studies of exchange scattering of electrons by helium, our knowledge of these cross sections is still rather fragmentary. Even in the reasonably high energy region the simple theory of the Born–Oppenheimer approximation seems to be inapplicable to exchange scattering. The recent investigations of Steelhammer and Lipsky (1970) show that the core contribution in the Born–Oppenheimer approximation depends strongly on the nature of the transition. Thus, whereas for the He $1^1S \rightarrow 2^3S$ transition the core contribution could not be neglected for energies below ~ 250 eV it was concluded by these authors that for transitions to P states of He, the core contribution at all energies could indeed be neglected except possibly at large scattering angles.

Joachain and Mittleman (1965) distinguished two problems in calculating electron–atom exchange scattering: the dynamical problem and the bound state problem; Joachain and Van den Eynde (1970) have shown the importance of including very accurately correlation effects in the target system.

In this paper, cross sections for excitation of helium from its ground state to the 2^3P and 3^3P excited states by electron impact have been obtained under the Ochkur approximation. Bound state effects in the present atomic rearrangement collision have also been investigated.

2. Theory

The cross section for excitation from the ground state of helium to a triplet state by electron impact may be written in the following form (Ochkur 1964).

$$Q_{\mathrm{on}} = \frac{24\pi}{k^6}\int_{K_{\min}}^{K_{\max}} |\langle\psi_n(\boldsymbol{r}_1, \boldsymbol{r}_2)|\, \mathrm{e}^{\mathrm{i}\boldsymbol{K}.\boldsymbol{r}_1}|\psi_0(\boldsymbol{r}_1, \boldsymbol{r}_2)\rangle|^2\, K\, \mathrm{d}K \tag{1}$$

where $\psi_0(\boldsymbol{r}_1, \boldsymbol{r}_2)$ and $\psi_n(\boldsymbol{r}_1, \boldsymbol{r}_2)$ are the wavefunctions for the ground and nth excited state of helium respectively.

$$K_{\text{min}} = k - k_{\text{on}}$$
$$K_{\text{max}} = k + k_{\text{on}}$$

where $\boldsymbol{k}$ and $\boldsymbol{k}_{\text{on}}$ are the momenta of the incident and outgoing electron respectively. All quantities are in atomic units, these units being employed throughout this paper unless otherwise mentioned.

3. Wavefunctions

3.1. Excited state wavefunction

The wavefunction employed in the present calculations to represent the helium excited state is the one given by Messmer (1969). These are written in the following form

$$\psi_n = \frac{1}{\sqrt{2}}\{\phi_{\text{s}}(1)\phi_{\text{p}}(2) - \phi_{\text{p}}(1)\phi_{\text{s}}(2)\} \tag{2}$$

ϕ_{s} and ϕ_{p} orbitals are represented as linear combinations of four basis functions in the following way

$$\phi_{\text{s}} = \sum_{n=1}^{4} c_{\text{s},n}\chi_{\text{s},n} \tag{3}$$

$$\phi_{\text{p}} = \sum_{n=2}^{5} c_{\text{p},n}\chi_{\text{p},n}. \tag{4}$$

The basis functions $\chi_{\text{s},n}$ and $\chi_{\text{p},n}$ are;

$$\chi_{\text{s},n} = \frac{(2\eta_{\text{s}})^{3/2}}{\{(2n)!\}^{1/2}}(2\eta_{\text{s}}r)^{n-1}\exp(-\eta_{\text{s}}r)Y_{0,0}(\theta, \phi) \tag{5}$$

$$\chi_{\text{p},n} = \frac{(2\eta_{\text{p}})^{3/2}}{\{(2n)!\}^{1/2}}(2\eta_{\text{p}}r)^{n-1}\exp(-\eta_{\text{p}}r)Y_{l,m}(\theta, \phi). \tag{6}$$

The parameters are taken from the paper of Messmer.

3.2. Ground state wavefunction

To describe the helium ground state we have used the following wavefunctions:

(i) An analytical fit to a Hartree–Fock wavefunction of Roothaan *et al* (1960) using a sum of two exponentials. In this form the wavefunction is written as

$$\psi_0(\boldsymbol{r}_1, \boldsymbol{r}_2) = \psi_0(r_1)\psi_0(r_2) \tag{7}$$

where

$$\psi_0(r) = \frac{N_{1\text{s}}}{\sqrt{\pi}}(\mathrm{e}^{-\alpha r} + \eta\,\mathrm{e}^{-\beta r})$$

For the parameters we have taken the values given by Byron and Joachain (1966), viz

$$\alpha = 1{\cdot}41, \beta = 2{\cdot}61, \eta = 0{\cdot}799, \text{and } N_{1\text{s}} = 1{\cdot}302525.$$

Results employing this wavefunction will be labelled by HF (BJ).

(ii) A 'configuration-interaction' wavefunction (Joachain and Vanderpoorten 1970) which takes account of angular correlations between the two electrons

$$\psi_0(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{1}{4\pi} \sum_{l=0}^{2} F_l(\boldsymbol{r}_1, \boldsymbol{r}_2) P_l(\cos\theta_{12}) \tag{8}$$

where

$$F_l(\boldsymbol{r}_1, \boldsymbol{r}_2) = \sum_{m \geqslant n} A_{mn}^{(l)} r_1^l r_2^l (r_1^m r_2^n + r_1^n r_2^m) \exp\{-\tfrac{1}{2}\beta(r_1 + r_2)\}.$$

Both m and n take values from 0 to 5 subject to the condition $m+n \leqslant 6$; thus there are 15 terms in each partial wave. Taking three partial waves and putting $\beta = 3{\cdot}7$, the ground state energy is given by $E_0 = -2{\cdot}9020$ au. Results employing this wavefunction will be denoted by JV.

4. Results and discussion

The values of the $1^1S \rightarrow 2^3P$ and $1^1S \rightarrow 3^3P$ electron impact excitation cross sections calculated by the Ochkur approximation are presented in table 1. We shall discuss the two excitation cross sections in turn.

Table 1. Excitation cross sections of triplet levels of helium in units of πa_0^2.

E (eV)	2^3P HF (BJ)	2^3P JV	3^3P HF (BJ)	3^3P JV
22	$0{\cdot}768^{-1}$†	$0{\cdot}600^{-1}$		
24	$0{\cdot}775^{-1}$	$0{\cdot}745^{-1}$	$0{\cdot}171^{-1}$	$0{\cdot}133^{-1}$
26	$0{\cdot}702^{-1}$	$0{\cdot}713^{-1}$	$0{\cdot}176^{-1}$	$0{\cdot}169^{-1}$
28	$0{\cdot}615^{-1}$	$0{\cdot}641^{-1}$	$0{\cdot}163^{-1}$	$0{\cdot}165^{-1}$
30	$0{\cdot}531^{-1}$	$0{\cdot}562^{-1}$	$0{\cdot}144^{-1}$	$0{\cdot}150^{-1}$
35	$0{\cdot}366^{-1}$	$0{\cdot}395^{-1}$	$0{\cdot}103^{-1}$	$0{\cdot}109^{-1}$
40	$0{\cdot}257^{-1}$	$0{\cdot}280^{-1}$	$0{\cdot}732^{-2}$	$0{\cdot}791^{-2}$
50	$0{\cdot}138^{-1}$	$0{\cdot}152^{-1}$	$0{\cdot}396^{-2}$	$0{\cdot}433^{-2}$
60	$0{\cdot}819^{-2}$	$0{\cdot}902^{-2}$	$0{\cdot}235^{-2}$	$0{\cdot}257^{-2}$
80	$0{\cdot}352^{-2}$	$0{\cdot}388^{-2}$	$0{\cdot}101^{-2}$	$0{\cdot}111^{-2}$
100	$0{\cdot}181^{-2}$	$0{\cdot}200^{-2}$	$0{\cdot}521^{-3}$	$0{\cdot}574^{-3}$
150	$0{\cdot}539^{-3}$	$0{\cdot}597^{-3}$	$0{\cdot}155^{-3}$	$0{\cdot}171^{-3}$
200	$0{\cdot}228^{-3}$	$0{\cdot}252^{-3}$	$0{\cdot}656^{-4}$	$0{\cdot}723^{-4}$
300	$0{\cdot}676^{-4}$	$0{\cdot}748^{-4}$	$0{\cdot}194^{-4}$	$0{\cdot}214^{-4}$
400	$0{\cdot}285^{-4}$	$0{\cdot}316^{-4}$	$0{\cdot}820^{-5}$	$0{\cdot}904^{-5}$
500	$0{\cdot}146^{-4}$	$0{\cdot}163^{-4}$	$0{\cdot}420^{-5}$	$0{\cdot}463^{-5}$

† The superscript denotes the power of ten by which the entry should be multiplied.

4.1. *Excitation of the 2^3P state*:

In figure 1 we compare our results with the results of the Born–Oppenheimer approximation calculated by Bell *et al* (1966), and also the results of the first order exchange approximation by the same authors. The results of elaborate calculations including exchange in the distorted wave approximation by Massey and Moiseiwitsch (1960),

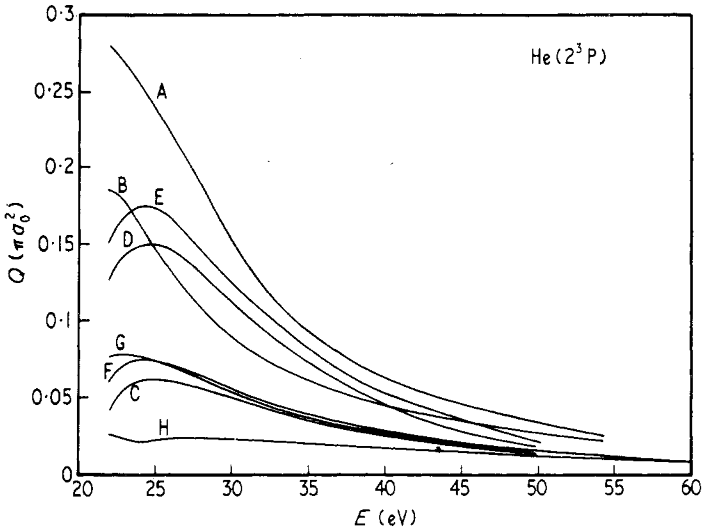

Figure 1. Cross sections for excitation of the 2^3P state of helium, A Born–Oppenheimer approximation (Bell *et al* 1966); B first order exchange approximation (Bell *et al* 1966); C Ochkur approximation (Ochkur *et al* 1965); D exchange distorted wave approximation (Massey *et al* 1960); E exchange distorted wave approximation (Lashmore–Davis 1965); F present work (JV); G present work (HF(BJ)); H experimental (Jobe *et al* 1967).

Lashmore-Davis (1965) and the results due to Ochkur and Brattsev (1965) together with the experimental data of Jobe and John (1967) have also been shown in figure 1.

We see that our HF (BJ) calculations are in fair accord with the calculations of Ochkur and Brattsev since they also used Hartree–Fock functions. Inspection of figure 1 shows that inclusion of correlation effects in the target wavefunctions does not bring agreement with the experimental results of Jobe *et al* at electron energy below about 30 eV. The cross section curves obtained with distorted wave approximation lies well above that given by Ochkur approximation. Moreover, the Born–Oppenheimer approximation overestimates such a cross section.

4.2. Excitation of the 3^3P state

From figure 2 we again find close agreement between our results and that of Ochkur and Brattsev for $E \geqslant 30$ eV. Our theoretical values agree with the recent experimental data due to McConkey and Woolsey (1969) for $E > 50$ eV, but the agreement becomes poor below this energy. The experimental cross sections corrected for polarization and cascading effects due to St John *et al* (1964) for electrons of various incident energies have also been presented in the figure 2. It is worth nothing that the values obtained by St John *et al*, are much larger than those of McConkey *et al* for higher values of incident electron energies.

Unfortunately, the experimental evidence on the excitation of the triplet states of helium does not form a coherent picture and hence no fruitful comparison with the theoretical results can be made.

Our results are based on very accurate ground state wavefunction, so that we have almost eliminated the bound state problem. Moreover, inspection of figures show that target effects do not affect the general shape of the cross section curve and are much more

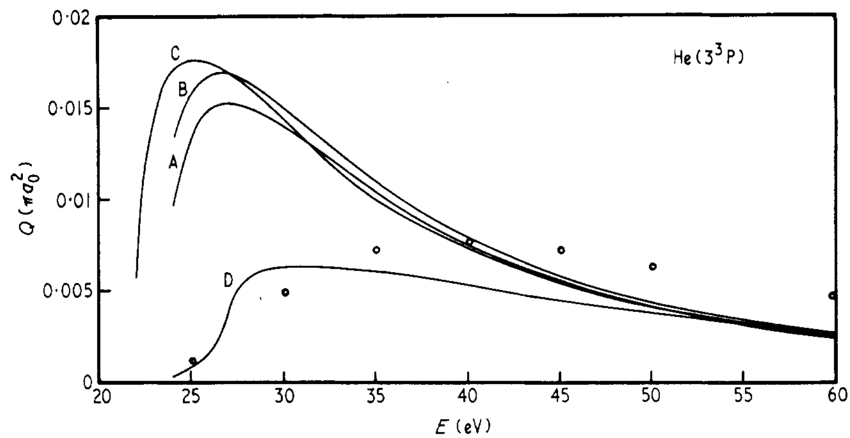

Figure 2. Cross sections for excitation of the 3^3P state of helium. A Ochkur approximation (Ochkur *et al* 1965); B present work (JV); C present work (HF(BJ)); D experimental (McConkey *et al* 1969); ○ experimental (John *et al* 1964).

pronounced in the lower energy region. This still leaves the dynamical problem to be taken care of, and the differences among the exchange cross sections calculated here can be attributed to differences in the theories.

Clearly more experimental work on the excitation of the 2^3P and 3^3P states of helium by electron impact is desirable.

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