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The simultaneous excitation and ionisation of helium by electron impact

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Abstract. Calculations for the process $e^- + He(1s^2\ ^1S) \rightarrow He^+(nl) + 2e^-$ where $n = 2$ are presented. The results are very different from previous calculations and show better agreement with experimental measurements of excitation to the 2p state. However, the theoretical calculations have an $E^{-1} \ln E$ behaviour for high incident energies E, while the experimental measurements appear to have an E^{-1} behaviour.

1. Introduction

Many calculations of electron impact ionisation have been reported in which the final-state ion is left in its ground state. By contrast the problem in which the final ion is left is an excited state has received relatively little attention, partly perhaps because experimental data for these processes are scarce. However Forand *et al* (1985) have reported an experiment in which the cross section for the process

$$e^- + He(1s^2\ ^1S) \rightarrow He^+(2p) + 2e^-$$

is measured. This experiment and an earlier measurement due to Bloemen *et al* (1981) indicate that near its maximum the cross section for producing 2^2P–1^2S emission in He^+ is about 6×10^{-19} cm^2. This value is in marked disagreement with existing theoretical values. Dalgarno and McDowell (1956) computed a peak value for this cross section of about 4×10^{-20} cm^2, while Gillespie (1972) found a corresponding value of 5.5×10^{-20} cm^2. Furthermore Forand *et al* (1985) show that their measured cross section has an E^{-1} high-energy behaviour and comment that 'this illustrates the optically forbidden nature of the simultaneous ionisation–excitation process as expected'. The discrepancy therefore between theory and experiment is very large and furthermore the observed energy dependence is not that which is to be expected on theoretical grounds.

The calculations of Dalgarno and McDowell (1956) and of Gillespie (1972) used plane waves to represent the scattered electron and simple uncorrelated wavefunctions to represent the atomic and continuum states. In this paper the cross section will first be evaluated using plane waves and a different choice of atomic states. This calculation demonstrates that it is the choice of atomic states that is of crucial importance in the calculation. It also shows explicitly the energy behaviour of the cross section and acts as a check case on a second, more elaborate, procedure. In this second method, as in the calculations of Jakubowicz and Moores (1981), wavefunctions generated in a close-coupling approximation are used to represent the final atomic state. The initial atomic state is represented by an analytic configuration interaction wavefunction.

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2. Theory

Let us use atomic units, except where otherwise specified, and consider the process in which an electron has an initial momentum $\boldsymbol{k}_0$ and collides with a normal helium atom which it ionises leaving the He^+ ion in a state labelled γ. The final electron momentum is $\boldsymbol{k}_0'$ and the momentum transfer is

$$\boldsymbol{q} = \boldsymbol{k}_0 - \boldsymbol{k}_0'.$$

If plane waves are used to describe the scattered electron then the scattering amplitude for this process is

$$f_\gamma(\boldsymbol{q}, \boldsymbol{k}_1) = -2q^{-2}\langle \Psi_\gamma^*(\boldsymbol{k}_1|\boldsymbol{r}_1\boldsymbol{r}_2)(e^{i\boldsymbol{q}\cdot\boldsymbol{r}_1} + e^{i\boldsymbol{q}\cdot\boldsymbol{r}_2})\Psi_0(\boldsymbol{r}_1\boldsymbol{r}_2)\rangle \tag{1}$$

where Ψ_0 is the normalised ground-state wavefunction of helium and Ψ_γ is a continuum state normalised so that

$$\langle \Psi_\gamma^*(\boldsymbol{k}_1|\boldsymbol{r}_1\boldsymbol{r}_2)\Psi_{\gamma'}(\boldsymbol{k}_1'|\boldsymbol{r}_1\boldsymbol{r}_2)\rangle = \delta_{\gamma\gamma'}\delta(\boldsymbol{k}_1 - \boldsymbol{k}_1'). \tag{2}$$

The total cross section for the excitation–ionisation process is given by

$$Q_{nl} = (\pi k_0)^{-1}\sum_m \int_0^{E_M} k_0' k_1 \mathrm{d}\left(\frac{k_1^2}{2}\right)\int |f_\gamma(\boldsymbol{q}, \boldsymbol{k}_1)|^2 \,\mathrm{d}\hat{\boldsymbol{k}}_1 \,\mathrm{d}\hat{\boldsymbol{k}}_0' \tag{3}$$

in units of πa_0^2, where $\gamma = (nlm)$, and $k_0'^2 + k_1^2 = 4E_M$ where

$$E_M = \tfrac{1}{4}[k_0^2 - 2I - 4(1 - n^{-2})] \tag{4}$$

I being the first ionisation energy of helium. In equation (3) all effects due to the identity of the incident electron with the atomic electrons have been ignored.

Let $F_{nl}(\alpha, r)$ be a normalised Sturmian function that satisfies the equation

$$F_{nl}''(\alpha, r) - \left(\alpha^2 - \frac{2n\alpha}{r} + \frac{l(l+1)}{r^2}\right)F_{nl}(\alpha, r) = 0. \tag{5}$$

Then a Coulomb approximation to the ground state is given by

$$\Psi_0(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{N}{4\pi}(r_1 r_2)^{-1}(1 + p_{12})F_{10}(2, r_1)F_{10}(1, r_2) \tag{6}$$

where N is the normalisation factor and p_{12} interchanges r_1 and r_2. The calculated ground-state energy using (6) is -2.841 au. The continuum state representing excitation to the 2p level can, in the same approximation, be written as

$$\Psi_\gamma(\boldsymbol{k}_1|\boldsymbol{r}_1, \boldsymbol{r}_2) = (4\pi^{3/2}k_1^{1/2}r_1 r_2)^{-1}(1 + p_{12})F_{21}(1, r_1)Y_{lm}(\hat{\boldsymbol{r}}_1)F_c(k_1, r_2) \tag{7}$$

where F_c has unit asymptotic amplitude and satisfies

$$F_c''(k_1, r) + (k_1^2 + 2r^{-1})F_c(k_1, r) = 0. \tag{8}$$

Using these wavefunctions the scattering amplitude is given by

$$f_\gamma(\boldsymbol{q}, \boldsymbol{k}_1) = -4Ni(\pi k_1^2)^{-1/2}q^{-2}\langle F_{10}(2, r_1)F_c(k, r_1)\rangle\langle F_{10}(1, r_2)F_{21}(1, r_2)j_1(qr_2)\rangle Y_{lm}(\hat{\boldsymbol{q}}) \tag{9}$$

where $j_\lambda(x)$ is a spherical Bessel function. In this picture the outer electron is excited into the final 2p state while the inner electron decays into the continuum. The only continuum partial wave that contributes is the s wave. All integrals can be performed analytically and the resulting cross section is

$$Q_{nl} = 32\left(\frac{N}{k_0}\right)^2 \int_0^{E_M} \mathrm{d}\left(\frac{k^2}{2}\right)\left(1 + \frac{k^2}{4}\right)^{-4}\left(\frac{e^{4\eta\theta_1}}{e^{2\pi\eta} - 1}\right)\int_{k_0 - k_0'}^{k_0 + k_0'} \frac{\mathrm{d}q}{q[1 + (q^2/4)]^6} \tag{10}$$

where $\eta = k^{-1}$ and

$$\theta_1 = \tfrac{1}{2}\tan^{-1}\left(\frac{4k}{k^2-4}\right) + \frac{\pi}{2}\varepsilon(2-k) \tag{11}$$

with ε denoting the unit step function.

It is apparent from (10) that at high energies

$$Q_{nl} \underset{k_0^2\to\infty}{\sim} k_0^{-2}(A \ln k_0^2 + B) \tag{12}$$

where A and B are constants.

In figure 1 the results given by (10) are compared with the results of Gillespie (1972), and differ at the cross section maximum by a factor of about 20; the comparison with the experiment of Forand *et al* (1985) shows that the maxima differ by a factor of 1.5 and that due to the value of A in (12) the shapes are very different. The calculation shows that the results are very sensitive to the choice of atomic wavefunctions and so these have been modified while plane waves have been retained to describe the scattered electron. The ground-state wavefunction has been represented by a configuration interaction generalisation of (6):

$$\Psi_0(\boldsymbol{r}_1\boldsymbol{r}_2) = (r_1 r_2)^{-1}(1+p_{12}) \sum_{ln_1n_2} a(ln_1n_2) F_{n_1 l}(\alpha_1 r_1) F_{n_2 l}(\alpha_2 r_2) y(ll0|\hat{\boldsymbol{r}}_1\hat{\boldsymbol{r}}_2) \tag{13}$$

where y denotes coupled spherical harmonics and the coefficients $a(ln_1n_2)$ are obtained using the program of Knox (1969). These wavefunctions have been used previously in line strength calculations (Knox and Rudge 1969). A number of different sized bases were used to assess the dependence of the cross section on the choice of basis. The results quoted were obtained using a two-configuration, thirteen-parameter wavefunction that gave a ground-state energy of -2.897 au.

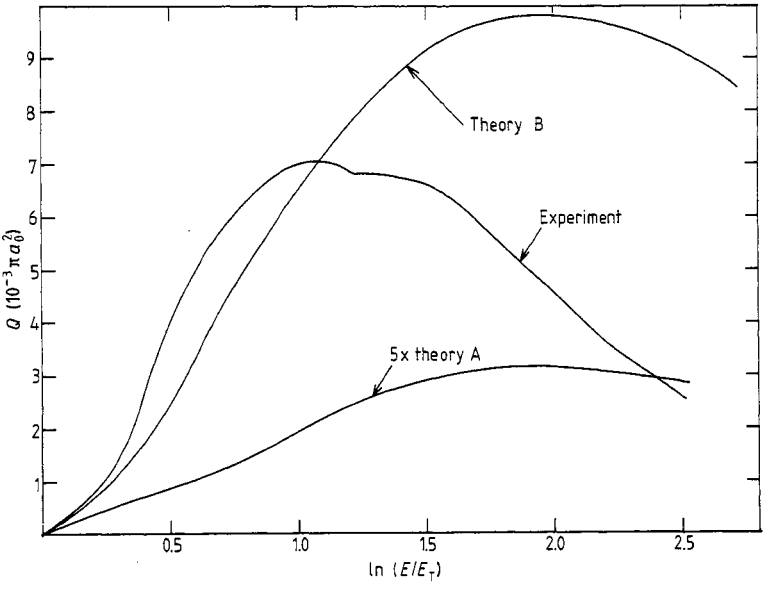

Figure 1. Cross sections for ionisation and excitation of the 2p state comparing the experimental values of Forand *et al* (1985) with theory A (Gillespie 1972) and equation (10), labelled theory B. E_T denotes the threshold energy, 65.38 eV.

The final atomic state was chosen to be a close-coupling generalisation of (7):

$$\Psi_\gamma(\boldsymbol{k}_1|\boldsymbol{r}_1\boldsymbol{r}_2)=(2/\pi k_1)^{1/2}\sum_{\substack{l_2m_2\\LM}}\exp[\mathrm{i}(\tfrac{1}{2}l_2\pi-\sigma_{l_2})]C^{l_1l_2L}_{m_1m_2M}Y_{l_2m_2}(\hat{\boldsymbol{k}}_1)\Psi^*_\Gamma(\boldsymbol{r}_1\boldsymbol{r}_2) \tag{14}$$

where $\Gamma=(n_1l_1l_2L)$ and $\sigma_{l_2}=\arg\Gamma(l_2+1-\mathrm{i}K_1^{-1})$. The function Ψ_Γ was obtained from the expansion

$$\Psi_\Gamma(\boldsymbol{r}_1,\boldsymbol{r}_2)=2^{-1/2}(1+p_{12})\sum_{\bar\Gamma}y(\bar l_1\bar l_2L|\hat{\boldsymbol{r}}_1\hat{\boldsymbol{r}}_2)F_{\bar n_1\bar l_1}(2,r_1)G_{\bar\Gamma\Gamma}(r_2). \tag{15}$$

The $G_{\bar\Gamma\Gamma}$ satisfy the usual close-coupling equations; 1s, 2s and 2p states of He^+ were included in the expansion. The equations were solved using an optimised iterative method and the solutions then fitted to allow the analytic evaluation of integrals. The matrix $\boldsymbol{G}$ which has as elements the solution $G_{\bar\Gamma\Gamma}$ satisfies the boundary condition

$$\boldsymbol{G}\underset{r\to\infty}{\sim}\sin\Theta\,\boldsymbol{k}^{-1/2}+(\exp\mathrm{i}\Theta)\boldsymbol{k}^{-1/2}\boldsymbol{T}. \tag{16}$$

In (16) $\boldsymbol{k}$ is the diagonal matrix that contains channel momenta k_j as elements and Θ is diagonal and contains Θ_j where

$$\Theta_j=k_jr-\tfrac{1}{2}l_j\pi+k_j^{-1}\ln(2k_jr)+\arg\Gamma(l_j+1-\mathrm{i}k_j^{-1}) \tag{17}$$

with l_j the channel angular momentum.

Using the functions (13) and (14) the total cross section is given by

$$Q_{nl}=32(\pi k_0^2)^{-1}\int_0^{E_M}\mathrm{d}\left(\frac{k^2}{2}\right)\int_{k_0-k_0'}^{k_0+k_0'}q^{-3}\sum_{l_2L}|T(nll_2L)|^2\,\mathrm{d}q \tag{18}$$

where

$$T(nll_2L)=\sum_{ln_1n_2\bar\Gamma}a(ln_1n_2)[\beta(\bar l_1\bar l_2lL)R_1^{l\bar\Gamma\Gamma}+\beta(\bar l_2\bar l_1lL)R_2^{l\bar\Gamma\Gamma}]. \tag{19}$$

In (19)

$$\beta(\bar l_1\bar l_2lL)=\delta_{l\bar l_2}(-1)^l(2\bar l_1+1)^{1/2}C^{\bar l_1lL}_{000} \tag{20}$$

and

$$R_t^{l\bar\Gamma\Gamma}=\langle F_{\bar n_1\bar l_1}(2,r_1)G_{\bar\Gamma\Gamma}(r_2)j_L(qr_t)(1+p_{12})F_{n_1l}(\alpha_1r_1)F_{n_2l}(\alpha_2r_2)\rangle. \tag{21}$$

The term $R_1^{l\bar\Gamma\Gamma}$ is an analogue of the simple expression (9) but, for excitation to a final 2p state, no longer contains just a continuum s wave because of the p-p, d-d... ground-state configurations. The term $R_2^{l\bar\Gamma\Gamma}$ represents excitation of one electron to the continuum with adjustment of the other electron to the final bound state. In both terms there is coupling between the 1s, 2s and 2p continua which is especially important for the channels associated with the two degenerate states. Resonance effects due to the existence of the higher-lying bound states are neglected in this calculation.

3. Results

Some calculated cross sections are shown in table 1 for simultaneous excitation and ionisation of the 2s and 2p states.

In the case of both final states the largest contribution to the cross section arises from $L=1$ but substantial contributions occur from $L=0$, 2 and some from higher L values. This means that at high energies the cross section again behaves like $Ak_0^{-2}\ln(k_0^2)$.

Figure 2 shows the experimental results of Moustafa Moussa and de Heer (1967), Bloemen *et al* (1981) and Forand *et al* (1985) and the theoretical results for excitation to the 2p state of He^+ and to the $n=2$ states. It can be seen that the more elaborate

Table 1. Computed total cross sections as a function of incident energy in units of $10^{-3}\ \pi a_0^2$.

Incident energy (eV)	Q_{2s}	Q_{2p}
100	1.02	2.10
150	1.94	3.24
200	2.45	3.31
300	2.28	2.92
500	2.01	2.94
750	1.94	1.73

calculation is in substantially better agreement with experiment than the calculations shown in figure 1. However, there is still a factor of two discrepancy between the calculations and the most recent experimental data. At high energies the calculated cross section disagrees in shape with the measured one. This is also clear from figure 3. If we write

$$Q_{nl} = \int_0^{E_M} \sigma_{nl}(k^2)\mathrm{d}\left(\frac{k^2}{2}\right) \tag{22}$$

then in figure 3 we show $k_0^2\sigma_{2p}(k^2)$ plotted against k, for three different initial energies. The increase as a function of k_0^2 gives rise to the logarithmic behaviour.

4. Concluding remarks

Ionisation without excitation is a large first-order transition and total cross sections for this process can be obtained quite accurately using simple wavefunctions. Ionisation with excitation has a much smaller probability and is correspondingly more difficult to calculate. The wavefunctions used here seem to be of adequate quality to produce

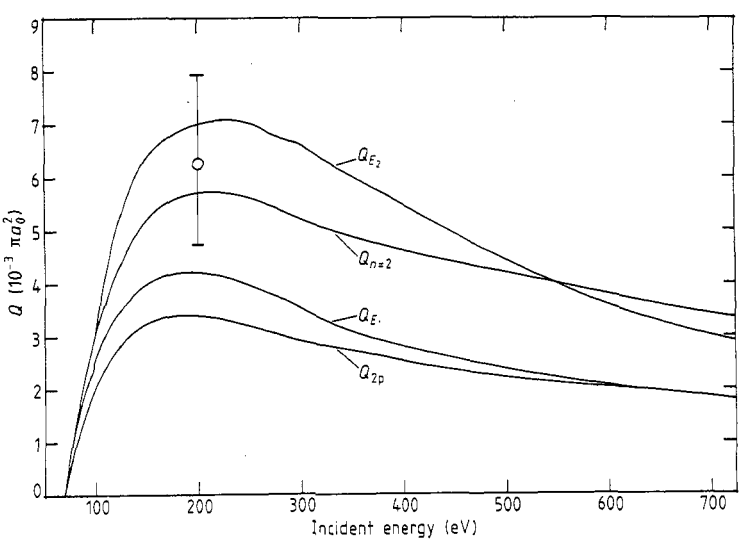

Figure 2. A comparison between the present calculations and the experimental measurements of Moustafa Moussa and de Heer (1967), Q_{E_1}, and Forand *et al* (1985), Q_{E_2}. $\bar{\bigcirc}$ denotes the measurement of Bloemen *et al* (1981) at 200 eV.

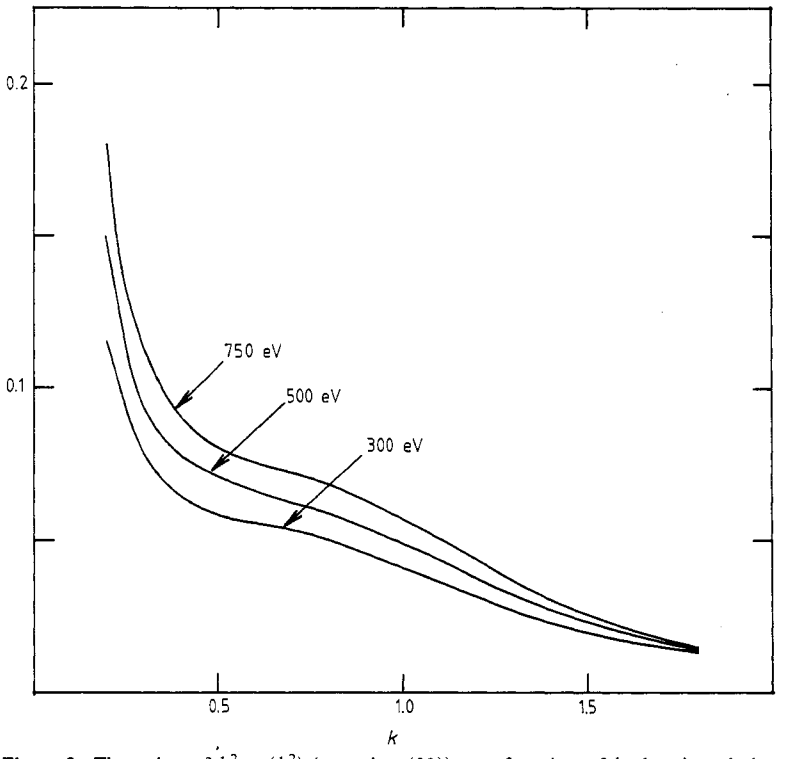

Figure 3. The value of $k_0^2\sigma_{2p}(k^2)$ (equation (22)) as a function of k, the ejected electron momentum, at three different incident energies.

a fairly accurate total cross section. There is an apparent difference at high energies between theory and experiment. The latter results could be reinterpreted as showing a small coefficient of the logarithmic term or it may be that the results, which are derived from a measurement of the intensity of the 2p-1s radiation, are partially obscured by cascade effects.

The principal result however is that an order of magnitude discrepancy between theory and experiment has been accounted for. Further improvements in the calculation can be made. The calculations show that the main contribution to the cross section arises from small momenta of the ejected electron and so exchange effects should not be large but may be significant at the lower energies. It may be important, at least insofar as the energy differential cross section is concerned, to include more He^+ states in the close-coupling expansion.

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