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Electron impact ionisation of helium at intermediate energies

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Abstract. Electron ionisation of helium at energies between 40 and 400 eV has been studied using a distorted-wave model based upon the assumption that the slower outgoing particle fully screens the residual ion. The model employs a consistent and elaborate description of all the channels involved. It appears that the present exchange model DWE agrees well with the measurements of the integrated ionisation cross section by Montague *et al.* The differences between DWE and experiment are of the same order of magnitude as the differences obtained by Campeanu *et al* in the positron impact case.

1. Introduction

Ionisation of helium by electron impact is a process for which accurate experimental integrated cross sections are available. The most accurate data are considered to be the recommended values of Montague *et al* (1984), which were the mean between the values obtained with the beam-gas cell technique (Rapp and Englander-Golden 1965) and those obtained with the fast crossed-beam technique (Montague *et al* 1984). While on the experimental side there is little doubt that these data are accurate, the progress on the theoretical side has been, and still is, very slow. Above approximately 500 eV there is reasonable agreement between measurements and the Bethe calculations of Kim and Inokuti (1971) and the Born results of Bell and Kingston (1969). At lower energies these two calculations are in good agreement with each other but are considerably higher than experiment.

There is no reliable theoretical calculation of the integrated cross section at low and medium energies. Most theoretical work (Madison *et al* 1977, Bransden *et al* 1979, Tweed 1980, Byron *et al* 1986, Mota Furtado and O'Mahony 1987) at low and intermediate energies has been directed towards obtaining differential cross sections in agreement with recent experiments. The only paper which gives distorted-wave integrated cross sections for intermediate energies is the one by Bransden *et al* (1979). They considered the distortion of all electron partial waves but in different ways. While the incident waves were computed with a second-order potential, the distortion of the outgoing waves was determined within an adiabatic approximation. They examined two models with different screening of the residual ion by the slower ejected electron. The results of the non-screening model are similar to the Born approximation values of Bell and Kingston (1969). The full-screening model produces results in good agreement with experiment above 250 eV but diverges at lower energies. Both approximations break down below 150 eV due to the use of the closure approximation.

By comparison the status of agreement between theory and experiment in positron impact ionisation of helium is much better. On the experimental side there are only integrated cross section measurements and there is considerable disagreement between the data obtained by the three experimental groups (Sueoka 1982, Diana *et al* 1985, Fromme *et al* 1986). The existing distorted-wave calculations (Campeanu *et al* 1987, hereafter referred to as I, and Basu *et al* 1985) clearly agree with the measurements of Fromme *et al* (1986). On the other hand, these theoretical papers show that for positron impact ionisation of helium even simple theoretical models can be in fairly good agreement with the experiment of Fromme *et al* (1986). The most elaborate distorted-wave calculation (model DCPE3 of I) is in excellent agreement with the experimental data for impact energies smaller than or equal to 60 eV, while for higher energies it yields cross sections about 5% larger than the experiment. Better agreement with the experiment can be obtained by using the 'truncated' version of DCPE3 (model DCPT3). Both DCPE3 and DCPT3 are based on the assumption that the slower outgoing particle fully screens the residual ion.

In the present work we examine the electron impact ionisation of helium by employing a model that is based on the same assumption (i.e. full screening of He^+ by the slower outgoing electron) and that uses the same complexity in the partial-wave representation as DCPE3. The complexity of the electron impact ionisation model is however increased relative to the positron work by the inclusion of electron exchange. In this way we can compare the effectiveness of this model in both electron and positron ionisation of helium. Since no experimental differential cross section data is currently available for positrons we cannot make a comparison at a more detailed level.

2. Theory

The distorted-wave formalism was explained in detail in I and hence we will point out only the new features related to electron impact ionisation.

Using the partial-wave expansions and performing the angular integrations, the e^- He ionisation total cross section (in units of πa_0^2) can be written as

$$Q(E_i) = \frac{16}{\pi E_i} \int_0^{E/2} dE_e \sum_{l_i l_e l_f} (2L+1) I(l_i l_e l_f) \tag{1}$$

where $I(l_i l_e l_f)$ is given by (Bransden *et al* 1979)

$$I(l_i l_e l_f) = \left| F - \frac{2l_e+1}{2(2l_f+1)} G^0 \right|^2 + \frac{3}{4} \left| \frac{2l_e+1}{2l_f+1} G^1 \right|^2. \tag{2}$$

In equations (1) and (2), l_i, l_e and l_f represent the orbital angular momentum quantum numbers of the incident, ejected and scattered electrons respectively, L is the total angular momentum quantum number, E_i the incident electron energy, $E = E_i - I = E_e + E_f$ is the total energy of the scattered electrons, where I is the ionisation energy, and E_e and E_f are the energies of the ejected and scattered electron respectively (all energies are in rydbergs).

Apart from the direct scattering amplitude F, written explicitly in I as a function of the channel radial wavefunctions, equation (2) also contains G^0 and G^1, the singlet and triplet exchange scattering amplitudes respectively. The singlet exchange amplitude G^0 is defined by the same expression as F but with the coordinates in the ejected and scattered wavefunctions interchanged. G^1 differs from G^0 by employing the triplet-state wavefunction for the two free electrons in the final channel instead of the singlet-state wavefunction.

Distorted-wave methods for electron ionisation have been used by a number of authors (Baluja and Taylor 1976, Bransden *et al* 1979, Madison *et al* 1977, Younger 1980). The model for the distortion of the ejected-electron wavefunction is the same as in I. It uses the distortion potential

$$V_e = V(e^-He^+; s+p+e) \tag{3}$$

where s, p and e stand for static potential, polarisation and electron exchange respectively. The polarisation potential of He^+ was calculated in the Bethe–Reeh model (Drachman and Temkin 1972), while exchange was included by antisymmetrising the total electronic wavefunction.

The bound-state He wavefunction is of the form used by Clementi and Roetti (1974). The incident-channel wavefunction is calculated in the polarised orbital approximation of McEachran *et al* (1977) employing a non-local distortion potential of the form

$$V_i = V(e^-He; s+p+e). \tag{4}$$

Since we assumed full screening by the slower ejected electron, the scattered electron channel wavefunction was calculated in the same manner as the incident wavefunction. The initial and final wavefunctions were not strictly orthogonal and this was taken into account in our calculation (cf § 3).

We shall denote by DWT the direct ionisation model:

$$I(l_i l_e l_f) = |F|^2 \tag{5}$$

while the exchange model, corresponding to equation (2), will be denoted by DWE. It should be noted that the upper limit in the integration in equation (1) is $E/2$, instead of E as in I. This modification, which is due to the indistinguishability of the two free electrons in electron impact ionisation problems, makes our model DWT look like DCPT3 of I.

The notation of our models is the same as that employed by Campeanu and Nagy (1985, 1986) in the ionisation of ionic targets by electron impact, although in those cases the radial scattering functions were calculated in the static approximation and $I(l_i l_e l_f)$ was obtained by using the 'maximum interference' model:

$$I(l_i l_e l_f) = |F|^2 + |G^0|^2 - |F||G^0|. \tag{6}$$

On the other hand, the work of Campeanu and Nagy used an exchange amplitude G^0 that was calculated by simply interchanging the energies of the scattered and ejected electrons in the direct amplitude F. This approximate method, while being less time consuming, yields integrated e^- He ionisation cross sections substantially higher than those obtained with our previous formulation. However, we expect that this approximation is less important for ionic targets than for neutral atomic targets.

3. Results and discussion

As in I, preliminary work established the most suitable mesh for the double radial integral of $I(l_i l_e l_f)$. The results presented in this paper correspond to the integration on a 158-point radial mesh extended to $r_{\max} = 18.7\ a_0$. However, one should note that if one assumes orthogonality between the initial and final states of the system (Campeanu and Nagy 1985, 1986), not only are the total cross sections slightly higher (about 3%), but also the convergence of the radial integration in $I(l_i l_e l_f)$ becomes worse and the truncation to 158 points becomes questionable. The energy integral in (1) was evaluated using 3-point Gaussian quadrature.

The convergence of $I(l_i l_e l_f)$ with the orbital angular momentum quantum numbers was found to be very similar to that in I and the reader is referred to that paper for

Table 1. Total cross sections for electron impact ionisation of helium calculated with our distorted-wave models. The results are given in units of πa_0^2.

Energy (eV)	DWT	DWE
40	0.2469	0.2217
60	0.4793	0.4189
80	0.5780	0.4767
100	0.5854	0.4750
120	0.5739	0.4648
150	0.5337	0.4408
200	0.4740	0.4011
250	0.4218	0.3631
300	0.3776	0.3308
400	0.3115	0.2846

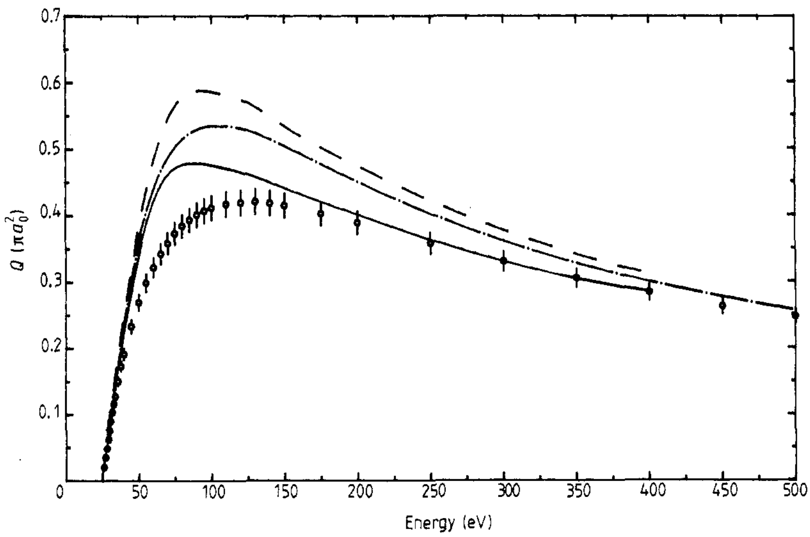

Figure 1. Comparison between the results obtained with various theoretical models and the experimental results. Theory: - - -, DWT; ——, DWE; — · —, Bell and Kingston (1969). Experiment: ○, Montague *et al* (1984).

numerical details. The maximum value for l_e was chosen to be 7, while the maximum for l_i varied from 10 for $E_i = 40$ eV to 50 for $E_i = 400$ eV. The values for l_f were found from the triangle condition.

Table 1 presents e^- He integrated ionisation cross sections corresponding to models DWT and DWE. Our theoretical results are compared in figure 1 with the experimental data of Montague *et al* (1984) and the modified Born (length) calculations of Bell and Kingston (1969). Both our models clearly show a maximum at an impact energy of about 100 eV; the exchange model being lower and in excellent agreement with the experiment for impact energies larger than 180 eV. However, as the impact energy decreases our model DWE produces data that are increasingly higher than the experimental data. The largest difference, obtained for 60 eV, is about 23%. It is also evident from figure 1 that the inclusion of exchange effects is more important than those of distortion.

It is interesting to compare the differences that exist between our theory and experiment for both electron and positron impact ionisation of helium. If one considers impact energies larger than about 100 eV the agreement is very similar for both cases. While at 100 eV the theoretical data are about 10% larger than the experimental data, the agreement becomes excellent around 200 eV. However, for impact energies below 100 eV the agreement improves in the positron impact case and deteriorates in the electron impact case.

4. Conclusions

The present paper investigates various models for calculating integrated ionisation cross sections for e^- He, by employing elaborate distorted-wave representations for all the partial waves of the ionising system. We assume in this approach that effects such as the correlation of the outgoing particles in the final state (i.e. energy, momentum and angular momentum exchange) are not too important and could be partially accounted for through our distortion models. The explicit inclusion of such effects seriously complicates the theory (Ehrhardt *et al* 1986).

Our data are very encouraging and indicate that our assumptions are reasonable. There is still some disagreement between our exchange model and the experiment at low energy, and for energies above 100 eV the disagreement is similar to the one noticed in the positron impact case.

The remaining disagreement, at low energies, with the highly accurate experimental results indicates that further refinements are necessary in our relatively simple model. Apart from the correlation effects, another possible source of error, for both the electron and positron impact cases, could be the representation of the bound-state He wavefunction (cf Mota Furtado and O'Mahony 1987, Tweed and Langlois 1987). In addition, the fact that for impact energies smaller than 100 eV the agreement with experiment in the electron case is worse than in the positron case might be explained by our neglect of the capture scattering amplitude (Ehrhardt *et al* 1986), which for low and intermediate impact energies is expected to be of the same order of magnitude as the exchange amplitude. We have also neglected the contribution due to autoionisation since there is no evidence of this in the experimental data, and hence we expect this contribution to the integrated cross section to be negligible.

In spite of these deficiencies our present model produces cross sections that agree very well with the experimental data at low and intermediate energies, and we are encouraged to continue to refine this model to produce even more reliable results and to extend it to differential cross sections.

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