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Positron Impact Ionisation of H and He Atoms: The Continuum Model*

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Abstract

The continuum optical potential model is used to calculate the ionisation cross sections of H and He by positron impact. The present e^+–H result is compared with the recent first measurement of e^+–H ionisation cross sections. The e^+–He calculation is also presented, together with the experimental measurements. A comparison with other theoretical results is also given.

1. Introduction

The long awaited positron scattering experiment on the H atom has been recently completed. Spicher *et al.* (1990) have reported the first measurements of positron impact ionisation of atomic hydrogen in the energy range 17·6 to 600 eV. Although there had been the earlier positron impact ionisation experiments on the He atom (Sueoka 1982; Diana *et al.* 1985; Fromme *et al.* 1986), this recent success is a major advancement in experimental positron–atom scattering. Naturally, it is hoped that we can look forward to more experimental measurements for e^+–H scattering in the future. A comprehensive review on current theoretical and experimental positron–atom collisions studies has been given by Charlton and Lariccha (1990).

The ionisation process for the e^+–H (as well as e^-–H) system involves a pure three-body Coulomb problem, which is intractable as a direct solution. Unlike the sophisticated *R*-matrix and coupled-channels-optical methods, which have achieved much success in studying electron–atom scattering (Fon *et al.* 1988; Bray *et al.* 1989), the theoretical progress in $e^\pm$–atom ionisation has been slow. Nevertheless, there are a number of distorted-wave techniques (Younger 1980, 1981) that have been successful to a certain extent.

Of the few theoretical calculations that have been made for the e^+–H and e^+–He ionisation processes, most have been based on the distorted-wave formalism. For the e^+–H case, there are the distorted-wave polarised orbital (DWPO) calculations of Ghosh *et al.* (1985) and the distorted-wave (DW) calculations of Mukherjee *et al.* (1989). Other calculations include the classical Monte Carlo trajectory-type methods of Ohsaki *et al.* (1985) and Wetmore and Olson (1986). All these calculations predict the qualitative shape shown by

* Dedicated to Professor Ian McCarthy on the occasion of his sixtieth birthday.

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the experimental cross sections. Generally, these methods predict lower cross sections than experiment, except at $E \leq 40$ eV where the results of Ghosh *et al.* and Mukherjee *et al.* show some agreement with the experimental data. In the e^+–He case, there are the detailed DW calculations of Campeanu *et al.* (1987) and Basu *et al.* (1985). In particular, Campeanu *et al.* have studied the effects of screening and distortion in their calculation of ionisation cross sections. Their best results show good agreement with the experimental data of Fromme *et al.* (1986).

Ian E. McCarthy has contributed much to the development of optical potential methods in electron–atom collision physics. The recent work of Bray *et al.* (1989) is another step forward in developing a complete *ab initio* optical potential model for electron–atom problems. The continuum optical method of McCarthy and Stelbovics (1980, 1983) can be described as a significant attempt to incorporate the continuum contribution into a coupled-channels framework. It does not include any empirical artefacts to describe physics. Nevertheless, it is an approximation to the exact three-body continuum problem. The justification in using this continuum optical model (COM) has been its ability to predict the electron-impact ionisation cross sections of atom and ions (McCarthy and Stelbovics 1983). The use of the continuum potentials in the coupled-channels-optical calculations of electron–atom collision processes has illustrated its significance (McCarthy *et al.* 1989; Ratnavelu and McCarthy 1990; Brunger *et al.* 1990).

It seems very much of theoretical interest to apply the COM for the e^+–H and e^+–H ionisation processes. We shall outline the essential features of this model in Section 2. The results and discussion will be presented in Section 3 and the conclusions in Section 4.

2. Theory and Formalism

A detailed description of the continuum optical potential model can be found in McCarthy and Stelbovics (1983). Here, we briefly outline the essential features of this method. The total ionisation cross section $\sigma_{\rm I}$ using the screening approximation (McCarthy and Stelbovics 1983) is given as

$$\sigma_{\rm I} = (2/k)(2\pi)^3 U(0)\,, \tag{1}$$

where $\boldsymbol{k}$ is the momentum of the incident positron and $U(0)$ is the imaginary part of the momentum-space optical potential $U(P)$ at momentum $P = 0$,

$$\begin{aligned} U(0) \;=\; & \pi \sum_{n_i} n_i \int \mathrm{d}^3 q_1 \int \mathrm{d}^3 q_2 \,\langle \boldsymbol{k}\phi_i \mid v \mid \chi^{(-)}(\boldsymbol{q}_<)\boldsymbol{q}_< \rangle \\ & \times \delta[E - \tfrac{1}{2}(q_1^2 + q_2^2)]\,\langle \boldsymbol{q}_> \chi^{(-)}(\boldsymbol{q}_<) \mid v \mid \phi_i \boldsymbol{k}\rangle\,. \end{aligned} \tag{2}$$

Here ϕ_i is the orbital for independent particle state i which is occupied by n_i electrons, E is the total energy, $\chi^{(-)}(\boldsymbol{q}_<)$ is a time-reversed Coulomb wave orthogonalised to ϕ_i, while $\boldsymbol{q}_<$ or $\boldsymbol{q}_>$ are respectively either $\boldsymbol{q}_1$ or $\boldsymbol{q}_2$ which ever has the lesser or greater magnitude, and v is the electron–positron potential. The contributions from heavy-particle knockout and autoionisation are neglected.

The extreme screening approximation (McCarthy and Stelbovics 1983) has been used, which for the e^+–H case should be

$$| \chi^{(+)}(\boldsymbol{q}_<)\boldsymbol{q}_>\rangle = | \boldsymbol{q}_1\rangle \chi(\boldsymbol{q}_2)_{z=-1} \text{ for } q_1 > q_2 \quad (3)$$

$$= \chi(\boldsymbol{q}_2)_{z=-2}\, \chi(\boldsymbol{q}_1)_{z=-1} \text{ for } q_2 > q_1 , \quad (4)$$

where the ejected 'fast' electron with momentum $\boldsymbol{q}_2$ sees an e^+–p effective charge of +2 and should be represented by a Coulomb wave with charge $z = -2$. Analytic forms for ionisation amplitudes using (4) are difficult to obtain. To perform a feasible calculation using the present programs without analytic expressions is a mammoth task and thus we approximate a plane wave for the 'fast' ejected electron. This is a high-energy approximation.

The amplitude for ionisation of an electron in an orbital ϕ_i resulting in a slow electron of momentum $\boldsymbol{p}$ and a fast positron of momentum $\boldsymbol{k}'$ is given by

$$\begin{aligned}\langle \boldsymbol{k}'\chi^{(-)}(\boldsymbol{p}) | v | \phi_i \boldsymbol{k}\rangle &= \langle \boldsymbol{k}\phi_i \mid v \mid \chi^{(+)}(\boldsymbol{p})\boldsymbol{k}'\rangle \\ &= (2\pi^2 K^2)^{-1} \int d^3q \,\langle \phi_i \mid q\rangle \\ &\times \left(\langle \boldsymbol{q} + \boldsymbol{K} \mid \psi^{(+)}(\boldsymbol{p})\rangle - \sum_m \langle \boldsymbol{q} + \boldsymbol{K} \mid \phi_{jm}\rangle\langle \phi_{jm} \mid \psi^{(+)}(\boldsymbol{p})\rangle \right), \quad (5)\end{aligned}$$

where $\boldsymbol{K} = \boldsymbol{k} - \boldsymbol{k}'$, $\psi^{(+)}(\boldsymbol{p})$ is a Coulomb wave and the magnetic degeneracies of the bound state ϕ_j are denoted by m (other quantum numbers for j are the same as for i).

In equation (5), the integral that has to be evaluated for the ionisation amplitudes is the Coulomb transform for the bound states (i or j) denoted as $C_i(\boldsymbol{k}, \boldsymbol{p})$. This is defined as

$$C_i(\boldsymbol{k}, \boldsymbol{p})\, Y^*_{lm}(\boldsymbol{p} - \boldsymbol{k}) = \int d\boldsymbol{q} \,\langle i \mid \boldsymbol{q}\rangle\langle \boldsymbol{q} + \boldsymbol{k} \mid \psi^{(+)}(\boldsymbol{p})\rangle, \quad (6)$$

where $Y_{lm}(\boldsymbol{p} - \boldsymbol{k})$ are spherical harmonics. The target state $\langle \boldsymbol{q} | i\rangle = \phi_i(\boldsymbol{q}) = R(q) Y_{lm}(\hat{\boldsymbol{q}})$. Then, we get

$$C_i(\boldsymbol{k}, \boldsymbol{p}) = \int d\boldsymbol{q} \,\langle R \mid \boldsymbol{q}\rangle\langle \boldsymbol{q} + \boldsymbol{k} \mid \psi^{(+)}(\boldsymbol{p})\rangle, \quad (7)$$

which is calculated by a method due to Belkić (1984), who had derived exact analytical forms for these integrals in spherical coordinates for Slater-type and hydrogenic orbitals. A detailed implementation of this procedure has been given by Ratnavelu (1989). This method has now superseded the very cumbersome procedure of Guth and Mullin (1951) (see McCarthy and Stelbovics 1980).

So, given the analytical approximations of the ionisation amplitudes, all that is needed is to evaluate the six-dimensional integral (2). This is done using the Diophantine multi-dimensional integration method (Conroy 1967).

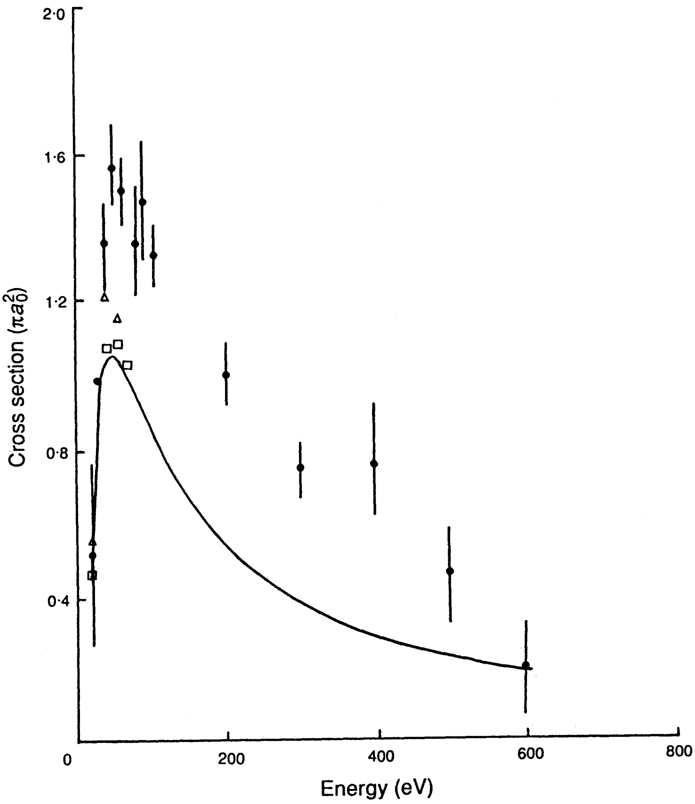

Fig. 1. Ionisation cross sections for e$^+$–H collisions. Experimental data (circles) are from Spicher *et al.* (1990); the curve is the COM; triangles are the DW1; and squares are the 'best' model of Mukherjee *et al.* (1989).

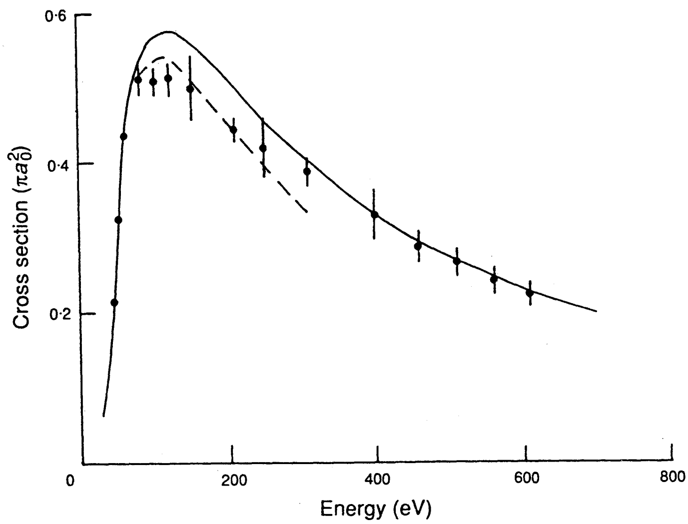

Fig. 2. Ionisation cross sections for e$^+$–He collisions. Experimental data (circles) are from Fromme *et al.* (1986); the solid curve is the COM; and the dashed curve is the DW calculation of Campeanu *et al.* (1987).

3. Results and Discussion

The cross sections for positron impact ionisation of the H atom (σ_{ion}^{+}) at energies 20·4–600 eV are depicted in Fig. 1. The cross sections calculated by the COM, the DW model 1 (DW1) of Ghosh *et al.* (1985) and the 'best' model of Mukherjee *et al.* (1989) are compared with the experimental data of Spicher *et al.* (1990). All the theoretical calculations predict a qualitative shape that is in fair agreement with experimental measurements. Furthermore, all calculations show good quantitative trends with experiment for $E \leq 40$ eV. For $40 < E \leq 60$ eV, the calculated cross sections are much smaller than the measurements. At energies between 60 and 500 eV, there are certainly large differences between the calculated and measured cross sections. This is quite puzzling as the COM is expected to reproduce ionisation cross sections better at higher energies. In comparison with electron impact ionisation of the hydrogen atom, the COM is a fairly good theoretical model (McCarthy and Stelbovics 1980; Ratnavelu and McCarthy 1990). At $E > 500$ eV, the theory begins to show a reasonable representation of experiment.

In the e^+–He case (see Fig. 2), the COM gives fairly good agreement with the measurements of Fromme *et al.* (1986) at most energies except between 80–200 eV. In comparison, the DW calculations of Campeanu *et al.* (1987) show much better agreement with experiment up to 250 eV. The DW calculations allow for screening and distortion effects which may explain the better agreement with experiment. At energies $E > 200$ eV, the COM reproduces the experimental data excellently.

4. Conclusions

The present calculation is an attempt to show the usefulness of the continuum optical potential model in calculating positron impact ionisation of atoms. Although the present COM results for the ionisation of the hydrogen atom may be a little disappointing for high energies, this difference between the COM and experiment may improve with further measurements in the future. It is premature to say that the COM is not working for e^+–H, when it does fairly well for the corresponding e^-–H (McCarthy and Stelbovics 1980). This argument is further strengthened with the good agreement between the COM and experiment for the e^+–He case.

In conclusion, the present method provides a useful and simple way of calculating positron impact ionisation of H and He at high energies. It may be useful in other positron impact–atom ionisation experiments.

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