Total Ionisation Cross Sections in $e^--H(2S)$ Scattering

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Abstract

Total cross sections for the electron impact ionisation from the 2S state of atomic hydrogen have been calculated in the energy range $5 \cdot 1-68$ eV of the incident electron by using a rigorous distorted wave method in which the effects of both the initial and final channel distortions are taken into account. The present results show improved agreement with experimental findings in comparison with other theoretical predictions.

1. Introduction

It has long been considered that ionisation in large current density gas discharges proceeds via stepwise ionisation of excited atoms by slower electrons, but a quantitative assessment of the problem has been precluded by a lack of reliable data on the ionisation of the excited atoms. The problem is of considerable practical interest in many industrial applications including fusion devices. Electron ionisation of atomic particles in excited states is also of fundamental importance in the elucidation of mechanisms in laboratory and astrophysical plasmas. It is therefore important to know both the functional form and the absolute magnitude of such cross sections.

Electron ionisation of excited states is studied here by using quantum mechanical approximations. The results include the ionisation cross section for the metastable 2S state of atomic hydrogen. This excited atom is the one most amenable to unambiguous experimental study because atomic hydrogen has only one metastable level and the metastable atoms can be readily produced and detected.

Rudge and Schwartz (1966) and Prasad (1966) calculated the total cross section (TCS) for the electron impact ionisation of the 2S state of atomic hydrogen using the Born-exchange (BE), Born-A and Born-B approximations. The problem has been studied experimentally by a number of workers. Koller

(1969) and Dixon *et al.* (1975) measured the TCS for e^- -H(2S) ionisation in the energy range $3 \cdot 4$ -10 eV and $8 \cdot 5$ -498 $\cdot 5$ eV respectively. But large error bars affect their data particularly at the low and high energy sides and their measurements also suffer from lack of data regarding the metastable population of the atomic beam. In order to remove these difficulties Defrance *et al.* (1981) studied the problem in the energy range $6 \cdot 3$ -998 $\cdot 5$ eV using a highly sophisticated experimental technique. They found that below an incident energy of 100 eV all experimental results are in mutual agreement and all the theoretical cross sections are much higher than the experimental ones, a situation similar to that of the ionisation of the ground state of atomic hydrogen by electron impact.

Recently Campeanu *et al.* (1988) have calculated the TCS for the electron impact ionisation of the ground state of helium by using a distorted wave model based on the assumption that the slower outgoing particle fully screens the residual ion. Their model employs a consistent and elaborate description of all the channels involved and their results including exchange are in excellent agreement with experimental findings. In the present paper we study the TCS for the electron impact ionisation of the 2S state of atomic hydrogen in the energy range $5 \cdot 1-68$ eV by using the distorted wave model of Campeanu *et al.* (1988).

2. Theory

The total cross section (TCS) for the electron impact ionisation of atomic hydrogen in the singlet and triplet modes is given by (Geltman 1969)

$$Q^{\pm} = \int d\mathbf{k}_2 d\hat{\mathbf{k}}_1 (k_1/k_0) |f_{\rm ion}^{\pm}(\mathbf{k}_1, \mathbf{k}_2)|^2, \qquad (1)$$

where \mathbf{k}_0 , \mathbf{k}_1 and \mathbf{k}_2 are the wavevectors of the incident, faster and slower electrons respectively. The superscripts (±) denote respectively the singlet and triplet spin states. The scattering amplitude $f_{ion}(\mathbf{k}_1, \mathbf{k}_2)$ for the ionisation of the atomic hydrogen in the 2S state is given by

$$f_{\text{ion}}(\mathbf{k}_1, \mathbf{k}_2) = (2\pi)^{-5/2} \int \chi^*_{\mathbf{k}_1}(z_1, \mathbf{r}_1) \chi^*_{\mathbf{k}_2}(z_2, \mathbf{r}_2) \\ \times V(r_1, r_2) \psi^{\pm}(\mathbf{r}_1, \mathbf{r}_2) \, d\mathbf{r}_1 \, d\mathbf{r}_2 \,, \qquad (2)$$

where $\chi_{k_1}(z_1, \mathbf{r}_1)$ and $\chi_{k_2}(z_2, \mathbf{r}_2)$ are the wavefunctions of the faster and the slower electrons, and z_1 and z_2 are respectively the effective charges seen by the faster and slower electrons. Following Campeanu *et al.* (1988) we have assumed the complete screening of the residual proton by the slower electron, i.e. we have taken $z_1=0$ and $z_2=1$. In our calculations the interaction potential is taken in the direct channel and is given by

$$V(r_1, r_2) = -\frac{1}{r_1} + \frac{1}{r_{12}},$$
(3)

In equation (2) the total wavefunction of the e⁻-H(2S) system is written as

$$\psi^{\pm}(\mathbf{r}_{1}, \mathbf{r}_{2}) = (1 \pm P_{12})\phi_{2S}(\mathbf{r}_{2})F^{\pm}(\mathbf{r}_{1}), \qquad (4)$$

where P_{12} is the permutation operator which interchanges the labels 1 and 2, and $\Phi_{2S}(\mathbf{r}_2)$ is the wavefunction of the 2S state of atomic hydrogen. The wavefunction of the incident electron and is decomposed into partial waves as

$$F^{\pm}(\mathbf{r}_{1}) = k_{i}^{-1/2} r_{1}^{-1} \sum_{l_{0}=0}^{\infty} (2l_{0}+1) i^{l_{0}} \exp(i \,\delta_{l_{0}}^{\pm}) \\ \times u_{l_{0}}(k_{0}, r_{1}) P_{l_{0}}(\cos \theta_{1}), \qquad (5)$$

where $\delta_{l_0}^{\pm}$ is the phase shift and $P_{l_0}(\cos\theta_1)$ is a Legendre polynomial.

The radial part $u_{l_0}^{\pm}(k_0, r_1)$ of $F^{\pm}(\mathbf{r}_1)$ satisfies the integro-differential equations corresponding to the static-exchange approximation (Bransden and Joachain 1983):

$$\left(\frac{d^2}{dr_1^2} - \frac{l_0(l_0+1)}{r_1^2} + k_0^2\right) u_{l_0}^{\pm}(k_0, r_1) = 2V_{2S,2S}(r_1) u_{l_0}^{\pm}(k_0, r_1) + r_1 R_{2S}(r_1) \left((E_{2S} - k_0^2) \delta_{l_00} \int_0^\infty R_{2S}(r_2) \right) \times u_{l_0}^{\pm}(k_0, r_2) r_2 dr_2 + \frac{2}{2l_0+1} \int_0^\infty R_{2S}(r_2) \times u_{l_0}^{\pm}(k_0, r_2) r_{l_0}(r_1, r_2) r_2 dr_2 \right),$$
(6)

where

$$V_{2S,2S}(r_1) = -\left(\frac{1}{r_1} + \frac{3}{4} + \frac{1}{4}r_1 + \frac{1}{8}\right)\exp(-r_1),\tag{7}$$

$$r_{l_0}(r_1, r_2) = \frac{r_{l_0}^{l_0}}{r_{l_0}^{l_0+1}},$$
(8)

and $r_{<}$ and $r_{>}$ are the lesser and greater of r_{1} and r_{2} . Further, $\delta_{l_{0},0}$ is the Kronecker delta, $R_{2S}(r)$ is the radial part of the wavefunction of the 2S state of atomic hydrogen, and E_{2S} is the energy of the 2S state of atomic hydrogen.

From equations (4) and (2) we can write

$$f_{\rm ion}^{\pm}(\mathbf{k}_1, \, \mathbf{k}_2) = f_{\rm d}^{\pm}(\mathbf{k}_1, \, \mathbf{k}_2) \pm f_{\rm e}^{\pm}(\mathbf{k}_1, \, \mathbf{k}_2), \tag{9}$$

where $f_d^{\pm}(\mathbf{k}_1, \mathbf{k}_2)$ and $f_e^{\pm}(\mathbf{k}_1, \mathbf{k}_2)$ are the direct and exchange scattering amplitudes respectively, and with

$$f_{d}^{\pm}(\boldsymbol{k}_{1}, \boldsymbol{k}_{2}) = (2\pi)^{-5/2} \int \chi_{\boldsymbol{k}_{1}}^{*}(z_{1}, \boldsymbol{r}_{1}) \chi_{\boldsymbol{k}_{2}}^{*}(z_{2}, \boldsymbol{r}_{2})$$
$$\times V(r_{1}, r_{2}) \Phi_{2S}(\boldsymbol{r}_{2}) F^{\pm}(\boldsymbol{r}_{1}) d\boldsymbol{r}_{1} d\boldsymbol{r}_{2} . \tag{10}$$

The exchange scattering amplitude has been obtained by invoking the Peterkop (1961) condition of exchange

$$f_{\rm e}^{\pm}(\boldsymbol{k}_1, \, \boldsymbol{k}_2) = f_{\rm d}^{\pm}(\boldsymbol{k}_2, \, \boldsymbol{k}_1). \tag{11}$$

Now since $z_2 = 1$, the slower electron is represented by a Coulomb wave in the field of the residual proton. The wavefunction $\chi_{k_2}(z_2, \mathbf{r})$ of the slower electron is decomposed into partial waves as

$$\chi_{\mathbf{k}_{2}}(z_{2}, \mathbf{r}) = 4\pi \sum_{l_{2}=0}^{\infty} \sum_{m_{2}=-l_{2}}^{l_{2}} i^{l_{2}} \frac{G_{l_{2}}(k_{2}r)}{k_{2}r} \times Y_{l_{2}m_{2}}(\hat{\mathbf{r}}) Y_{l_{2}m_{2}}^{*}(\hat{k}_{2}) \exp\{-i\eta_{l_{2}}(k_{2})\}, \qquad (12)$$

where $G_{l_2}(k_2 r)$ is the regular Coulomb function of order l_2 and $\eta_{l_2}(k_2)$ is the Coulomb phase shift (Abramowitz 1972).

Since we have assumed the complete screening of the residual proton by the slower electron, the wavefunction of the faster electron is calculated in the same manner as that of the incident electron (Campeanu *et al.* 1988). We have carried out the partial wave analysis of $f_{ion}^{\pm}(\mathbf{k}_1, \mathbf{k}_2)$. Now the TCS for ionisation for an unpolarised beam of incident electrons is given by

$$Q = \frac{1}{4}Q^{+} + \frac{3}{4}Q^{-}.$$
 (13)

Table 1. Total cross section Q (in units of πa_0^2) for e⁻-H(2S) ionisation

Incident electron energy E_0 (eV)	Q
5.1	4.656
7.65	8.416
10.2	10.03
13.6	9-424
17.0	8.672
20-4	7.968
30.6	6.608
40.8	5-360
54-4	4-432
68.0	3.792

3. Results and Discussions

The radial integrals occurring in the expression for Q have been evaluated up to a radial distance of 80 a.u. using 16-point Gauss-Legendre quadrature. The integro-differential equations satisfied by $u_{l_0}^{\pm}(k_0, r_1)$ have been solved by using the Numerov method (Sloan 1964) with a stepsize of 0.02 a.u. up to a radial distance of r = 40 a.u. The Coulomb function $G_{l_2}(k_2 r)$ was obtained by solving the corresponding differential equation with a step size of 0.02 a.u. The integral over k_2 in the expression for Q has been evaluated by 8-point Gauss-Legendre quadrature. The maximum value of l_2 in the sum over l_2 in the expression for Q has been taken as 5. The maximum value of l_0 has been varied from 11 for $E_0 = 5 \cdot 1$ eV (the energy of the incident electron) to $l_0 = 20$ for $E_0 = 68$ eV. The value of l_1 has been obtained by using the triangle rule involving l_0 , l_1 and l_2 [i.e. $|l_0 - l_2| \le l_1 \le (l_0 + l_2)$].

As a check of our computer code we have reproduced the following results: (i) the Born-A and Born-B results of Prasad (1966) and (ii) the Born-exchange (BE) results of Rudge and Schwartz (1966). In Fig. 1 we plot our present results together with the BE results of Prasad (1966), the BE results of Rudge and Schwartz (1966) and the experimental results of Defrance *et al.* (1981). Table 1 summarises our present results. On comparing our results with those of Prasad (1966) and Rudge and Schwartz (1966) we find that the present distorted wave model produces an improved agreement with the experimental results in the energy region considered. It also shows the importance of initial and final distortion in $e^--H(2S)$ ionisation in agreement with the findings of Campeanu *et al.* (1988) in the case of e^- -He ionisation.



Fig. 1. Total cross section Q in units of 10^{-16} cm² for e⁻-H(2S) ionisation: curve A, BE results of Rudge and Schwartz (1966); curve B, BE results of Prasad (1966); and curve C, present distorted wave results. The experimental results are from Defrance *et al.* (1981).

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