Aust. J. Phys., 1996, **49**, 937–44

Electron Impact Ionisation of Metastable 2s-state Hydrogen Atoms

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Abstract

The triple differential cross section for ionisation of hydrogen atoms in the metastable 2s-state by electrons of 250 eV incidence energy has been calculated following the multiple scattering theory of Das and Seal (1993). The results are compared with the first Born results and with the results of some other theories. Additional features are noted in the cross section curves of the present calculation. These offer wider scope for the experimental study of ionisation of hydrogen atoms in their metastable states.

1. Introduction

At present there exist many theoretical calculations of cross sections for ionisation of hydrogen atoms in the ground state at various incident energies and under different kinematic conditions (see for example Byron and Joachain 1989; Lahmam-Bennani 1991; Ehrhardt *et al.* 1988; Das and Seal 1993, 1994; Konovalov 1994). Ionisation of hydrogen atoms by electrons is the fundamental and simplest ionisation problem. On different counts its theoretical study is important. The availability of huge amounts of experimental data makes the field more interesting. New developments are still being observed in this field (see Kato and Watanabe 1995; Das 1994). Unfortunately, in comparison, ionisation from excited states has not been investigated to the same extent. This is mainly due to the absence of any experimental activity on these problems. It now appears that the investigation of ionisation from metastable states of hydrogen atoms by charged particles is equally interesting and the time is not far off when experimental results will be available in this field. At present, beyond the first Born results there exists the second Born calculation of Vučič *et al.* (1987) and the BBK calculation of Hafid *et al.* (1993) for small momentum transfer asymmetric scattering at 250 eV for the incident electron. Here we add to the existing theoretical results a few new sets of theoretical data from a calculation following the multiple scattering theory of Das and Seal (1993). It may be noted that this multiple scattering theory gives good cross section results for the ionisation of hydrogen (Das and Seal 1993) and helium atoms (Das and Seal 1994) in their ground states, so the present results for ionisation from the 2s state may also be expected to be good. The present calculation reveals new features in the cross section curves which may be confirmed by experiments.

0004-9506/96/050937$05.00

2. Theory

The multiple scattering theory of ionisation of hydrogen atoms by electrons is described in detail in the paper by Das and Seal (1993). Here we describe the method very briefly, particularly for clarification of the notation. The T-matrix element for direct scattering is given by

$$T_{\mathrm{fi}} = \langle \Psi_{\mathrm{f}}^{(-)} | V_{\mathrm{i}} | \Phi_{\mathrm{i}} \rangle \,, \tag{1}$$

where

$$\Phi_{\mathrm{i}}(\boldsymbol{r}_1, \boldsymbol{r}_2) = \phi_{2\mathrm{s}}(r_1)\, \mathrm{e}^{\mathrm{i}\boldsymbol{p}_{\mathrm{i}} \cdot \boldsymbol{r}_2} / (2\pi)^{\frac{3}{2}} \,,$$

$$V_{\mathrm{i}}(\boldsymbol{r}_1, \boldsymbol{r}_2) = 1/r_{12} - 1/r_2 \,,$$

and where $\phi_{2\mathrm{s}}(\boldsymbol{r}_1)$ is the hydrogenic 2s wavefunction, $\boldsymbol{p}_{\mathrm{i}}$ is the incident electron momentum, E_{i} is its energy and $\Psi_{\mathrm{f}}^{(-)}(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is the final three-particle scattering state with the electrons being in the continuum with momenta $\boldsymbol{p}_1$, $\boldsymbol{p}_2$ and energies E_1, E_2 respectively. Coordinates of the two electrons are taken to be $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$. Here $\Psi_{\mathrm{f}}^{(-)}(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is approximated by a wavefunction $\Psi_{\mathrm{f}}^{0(-)}$ given by (Das and Seal 1993)

$$\Psi_{\mathrm{f}}^{0(-)}(\boldsymbol{r}_1, \boldsymbol{r}_2) = N(\boldsymbol{p}_1, \boldsymbol{p}_2)[\phi_{\boldsymbol{p}_1}^{(-)}(\boldsymbol{r}_1)\mathrm{e}^{\mathrm{i}\boldsymbol{p}_2 \cdot \boldsymbol{r}_2} + \phi_{\boldsymbol{p}_2}^{(-)}(\boldsymbol{r}_2)\mathrm{e}^{\mathrm{i}\boldsymbol{p}_1 \cdot \boldsymbol{r}_1}$$
$$+ \phi_{\boldsymbol{p}}^{(-)}(\boldsymbol{r})\mathrm{e}^{\mathrm{i}\boldsymbol{p} \cdot \boldsymbol{R}} - 2\mathrm{e}^{\mathrm{i}\boldsymbol{p}_1 \cdot \boldsymbol{r}_1 + \mathrm{i}\boldsymbol{p}_2 \cdot \boldsymbol{r}_2}]/(2\pi)^3 \,, \tag{2}$$

where

$$\boldsymbol{r} = (\boldsymbol{r}_2 - \boldsymbol{r}_1)/2 \,, \qquad \boldsymbol{R} = (\boldsymbol{r}_2 + \boldsymbol{r}_1)/2 \,,$$

$$\boldsymbol{p} = (\boldsymbol{p}_2 - \boldsymbol{p}_1) \,, \qquad \boldsymbol{P} = (\boldsymbol{p}_2 + \boldsymbol{p}_1) \,.$$

Here $\phi_q^{(-)}(\boldsymbol{r})$ is the Coulomb wavefunction given by

$$\phi_q^{(-)}(\boldsymbol{r}) = \mathrm{e}^{\pi\alpha/2}\Gamma(1 + \mathrm{i}\alpha)\mathrm{e}^{\mathrm{i}\boldsymbol{q} \cdot \boldsymbol{r}}\, {}_1F_1(-\mathrm{i}\alpha, 1, -\mathrm{i}[qr + \boldsymbol{q} \cdot \boldsymbol{r}]) \,,$$

where $\alpha = 1/p_1$ for $\boldsymbol{q} = \boldsymbol{p}_1$, $\alpha = 1/p_2$ for $\boldsymbol{q} = \boldsymbol{p}_2$ and $\alpha = -1/p$ for $\boldsymbol{q} = \boldsymbol{p}$.

The normalisation constant $N(\boldsymbol{p}_1, \boldsymbol{p}_2)$ is given by

$$|N(\boldsymbol{p}_1, \boldsymbol{p}_2)|^{-2} = |7 - 2[\lambda_1 + \lambda_2 + \lambda_3] - [2/\lambda_1 + 2/\lambda_2 + 2/\lambda_3]$$
$$+ [\lambda_1/\lambda_2 + \lambda_1/\lambda_3 + \lambda_2/\lambda_1 + \lambda_2/\lambda_3 + \lambda_3/\lambda_1 + \lambda_3/\lambda_2]| \,, \tag{3}$$

where

$$\lambda_1 = \mathrm{e}^{\pi\alpha_1/2}\Gamma(1 - \mathrm{i}\alpha_1) \,, \qquad \alpha_1 = 1/p_1 \,,$$

$$\lambda_2 = \mathrm{e}^{\pi\alpha_2/2}\Gamma(1 - \mathrm{i}\alpha_2) \,, \qquad \alpha_2 = 1/p_2 \,,$$

$$\lambda_3 = \mathrm{e}^{\pi\alpha}\Gamma(1 - \mathrm{i}\alpha) \,, \qquad \alpha = -1/p \,.$$

Most of the integrals which occur in the T-matrix elements may be exactly evaluated. The few remaining integrals can be reduced to one-dimensional integrals.

These are numerically evaluated using the Gaussian quadrature formula. The direct scattering amplitude is then calculated from

$$f(\boldsymbol{p}_1, \boldsymbol{p}_2) = -(2\pi)^2 T_{\mathrm{fi}}\,, \tag{4}$$

and the exchange amplitude is approximated by

$$g(\boldsymbol{p}_1, \boldsymbol{p}_2) = f(\boldsymbol{p}_2, \boldsymbol{p}_1)\,. \tag{5}$$

The triple differential cross section is finally given by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega_1\,\mathrm{d}\Omega_2\,\mathrm{d}E_1} = \frac{p_1 p_2}{p_i}\left[\tfrac{3}{4}|f-g|^2 + \tfrac{1}{4}|f+g|^2\right]. \tag{6}$$

3. Results

The triple differential cross section results of our calculation are presented in Figs $1a$–$1f$ for scattering in a plane. Here the incident electron energy is $E_{\mathrm{i}} = 250$ eV, the ejected electron energy is $E_1 = 5$ eV and the scattering angles are $\theta_2 = 5°$ ($1a$), $7°$ ($1b$), $9°$ ($1c$), $11°$ ($1d$), $15°$ ($1e$) and $20°$ ($1f$) and the ejection angle θ_1 varies from $0°$ to $360°$ (measured oppositely from the forward direction compared to that for scattering angle θ_2). We also include here the first Born results and, whenever available, those of the second Born and BBK calculations. For $\theta_2 = 5°$ (Fig. $1a$) there are gross differences among the results of various calculations. The binary peak value of the present calculation is lowest among all calculations and is about half of that of the first Born calculation. In the 'recoil region', instead of peaks (as in other calculations) there is a strong minimum. The minimum value is about two orders smaller than results of other calculations. For $\theta_2 = 7°$ (Fig. $1b$) there is also a strong minimum in the recoil region. Here the first Born calculation gives a flat minimum while the second Born shows slight fluctuations in the cross section values. For this case the binary peaks of all calculations practically coincide with each other. For $\theta_2 = 9°$ (see Fig. $1c$) the cross section curve of the present calculation changes shape in the recoil region. Here the minimum is less pronounced and moves to a larger angle, and a peak develops between the forward direction and the minimum. The binary peak in this case becomes the most strong and sharp. As the scattering angle θ_2 increases the peak height again decreases.

The characteristic features of the cross section curve of the present calculation slowly change as the scattering angle increases further (see Figs $1d$, $1e$ and $1f$). For larger scattering angles, the results of the present calculation are many times larger than the first Born results. All these results offer good scope for the experimental investigation of these problems and offer a new test for different theories of ionisation.

We present the binary peak values against the corresponding scattering angles in Fig. 2. Here it is clear that the peak values of the present calculation agree with the first and second Born results only in the interval $6°$–$9°$, say. Outside this interval there are gross differences, the present results being the minimum. Beyond $15°$ the binary peak value of the present calculation becomes larger than that of

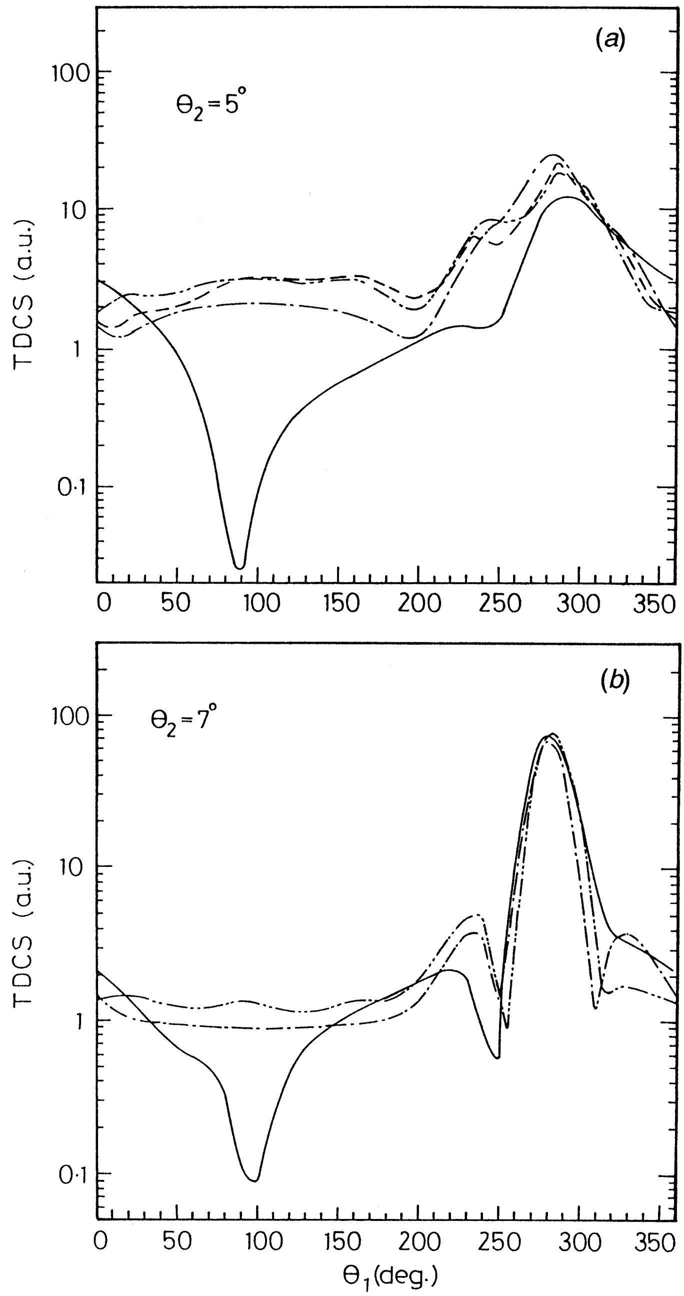

Fig. 1. Triple differential cross section versus ejection angle θ_1 for electron impact energy $E_i = 250$ eV, ejected electron energy $E_1 = 5$ eV and for scattering angles $\theta_2 = 5°$ (1*a*), 7° (1*b*), 9° (1*c*), 11° (1*d*), 15° (1*e*) and 20° (1*f*). Continuous curve, present calculation; dash–dot curve, first Born approximation; dash–double-dot curve, second Born calculation; and dashed curve, BBK theory.

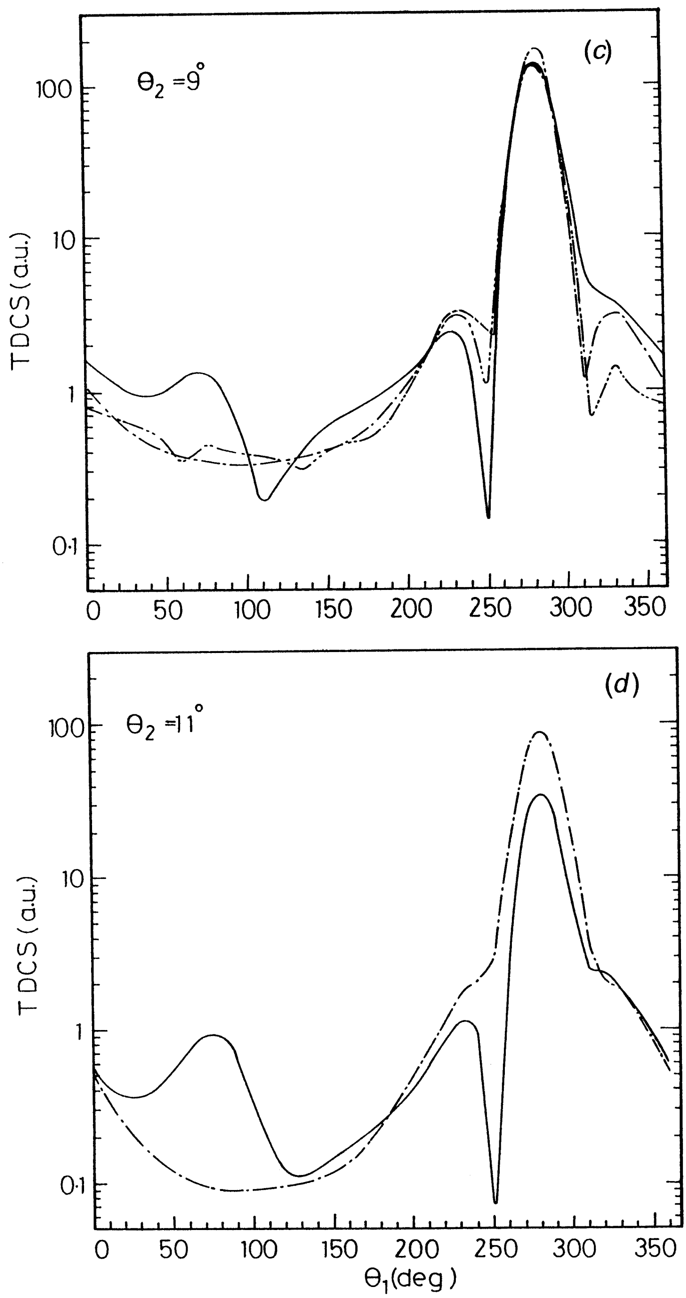

Fig. 1 (*Continued*)

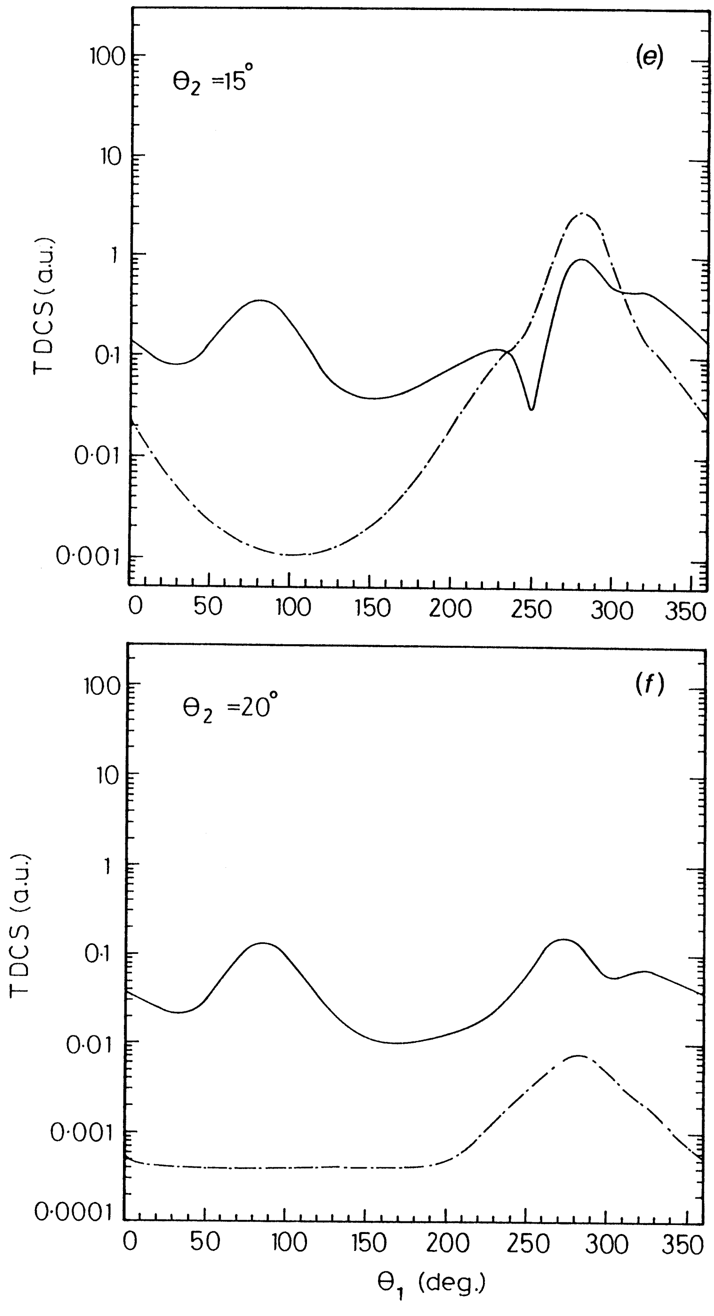

Fig. 1 (*Continued*)

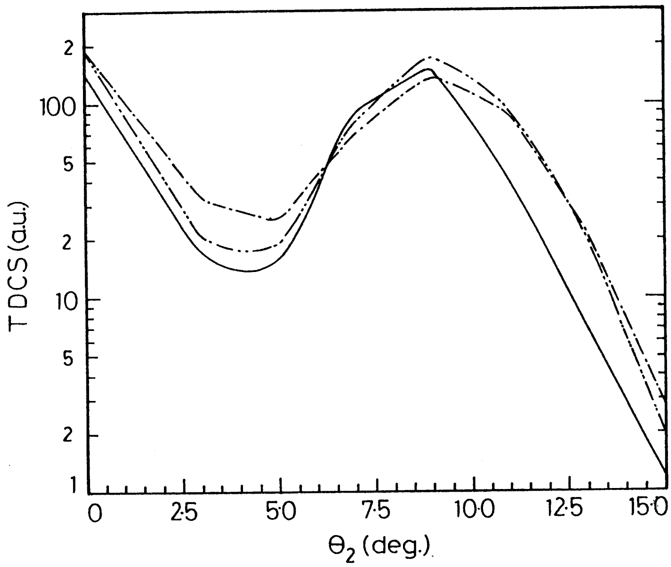

Fig. 2. Binary peak values versus peak angles for the triple differential cross section for electron impact energy 250 eV and ejected electron energy 5 eV. Continuous curve, present calculation; dash–dot curve, first Born calculation; and dash–double-dot curve, second Born calculation.

the first Born calculation. Experimental measurements of the peak values will give an additional test of the validity of different theories.

4. Conclusions

The present calculation reveals additional possible features of the cross section curves for small momentum transfer in the ionisation of the hydrogen atom in the metastable 2s state by 250 eV electron impact. New experimental results will be valuable and will add a new dimension to the study of the ionisation problem. Calculations for other kinematic conditions or for other atomic species will also be interesting.

Acknowledgments

The author is grateful to Professor J. N. Das for giving research guidance and under whose supervision the present work was completed. He extends his gratitude to the Indian Council for Cultural Relations (ICCR) for financial support. He is also thankful to the Head of the Department of Applied Mathematics, Calcutta University.

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Manuscript received 9 January, accepted 28 March 1996