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TOTAL CROSS SECTION FOR ($e^- - \mathrm{H}(1S)$) IONIZATION

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The total cross section for the electron impact ionization of the ground state of atomic hydrogen has been calculated in the energy range 20.4 – 68 eV using a rigorous distorted wave method in which the effects of target and final channel distortions are taken into account. The present results are compared with the experimental and other theoretical results.

I. INTRODUCTION

For many years there has been a considerable interest in the electron impact ionization process, both from the fundamental point of view of how to develop reliable methods to calculate a total cross section (TCS) as well as from the practical need to obtain accurate data for plasma and fusion research [1]. In the case of the electron impact ionization of atomic hydrogen there have been a number of experimental measurements [2—5] of total cross sections. Recently Shah et al. [6] have measured the TCS for the $e^- - \mathrm{H}(1S)$ ionization using a pulsed cross beam technique. Although different experimental results are close to each other the theoretical predictions of TCS for low and intermediate energies differ appreciably from the experimental results.

Rudge and Schwartz [7] studied the problem in the energy range of 20.4 – 68 eV of the incident electron using the Born-Exchange (BE) approximation in which the Peterkop condition [8] of exchange was employed. Their theoretical predictions are higher than the measured values. Golden and McGuire [9] computed the total cross sections (TCS) for the process using

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the Glauber approximation in the energy range of 17 – 95 eV. At low energies their results including the exchange lie below the experimental results. They themselves have remarked that in the low energy range there is no rigorous justification for their results. There have been a few pseudostate calculations of ionization [10, 11] in which the ionization cross section has been evaluated by determining the fraction of each pseudostate lying in the continuum and then adopting the assumption that the ionization cross section is equal to the pseudostate excitation cross section times this fraction summed over pseudostates. It is noteworthy that the calculated cross sections tend be on the lower side of experimental results particularly at high energies.

Recently Campeanu et al. [12] have calculated the TCS for the electron impact ionization of helium using a distorted wave model based upon the assumption that the slower outgoing particle fully screens the residual ion. Their models employ a consistent and elaborate description of all the channels involved. Their results are in excellent agrement with experimental findings. In the present paper we have applied the distorted wave model of Campeanu et al. [12] to study the TCS for the electron impact ionization of atomic hydrogen in the energy range of 20.4 – 68 eV. We have also taken into account the effect of the target distortion, i.e. the distortion of the electron cloud of the target atomic hydrogen by the incoming electron [13, 14] in our distorted wave model. This effect has been found to be important in the electron — hydrogen scattering [15].

II. THEORY

Let $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ be the position vectors of the incident and the target electron with respect to the proton which is assumed to be at rest in the origin of the co-ordinate system. Taking into account the effect of target distortion the total wave function for the system of the incident electron and the hydrogen atom is given by [16, 17],

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = (1 \pm P_{12})[\Phi_{1s}(\boldsymbol{r}_2) + \Phi_d(\boldsymbol{r}_1, \boldsymbol{r}_2)]F^{\pm}(\boldsymbol{r}_1). \tag{1}$$

Where P_{12} permutes the electron labels 1 and 2. $\Phi_{1s}(\boldsymbol{r})$ is the wave function of the ground state of atomic hydrogen. $\Phi_d(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is the first order perturbation due to distortion induced in the target by the presence of the incident electron. It assumes the form [16, 17].

$$\Phi_d(\boldsymbol{r}_1, \boldsymbol{r}_2) = -\pi^{-1/2} \frac{\varepsilon(r_1, r_2)}{r_1^2} \frac{\eta_{1s\to p}(r_2)}{r_2} P_1(\cos(\hat{r}_1 . \hat{r}_2)), \tag{2}$$

where

$$\varepsilon(r_1, r_2) = \begin{cases} 1 & r_1 > r_2 \\ 0 & r_1 < r_2 \end{cases} \tag{3}$$

and

$$\eta_{1s\to p}(r) = \left(\frac{1}{2} r^3 + r^2\right) \exp(-r). \tag{4}$$

The superscripts $(\pm)$ stand for the singlet and the triplet spin states

$$\Phi_{1s}(\boldsymbol{r}) = R_{1s}(r) Y_{00}(\hat{r}). \tag{5}$$

$R_{1s}(r)$ is the radial part of the wave function of the hydrogen atom in the ground state. The distorted wave $F^{\pm}(\boldsymbol{r}_1)$ describing the incoming electron is decomposed into partial waves at

$$F^{\pm}(\boldsymbol{r}_1) = k_i^{-1/2} \sum_{l_i=0}^{\infty} (2l_i + 1) i^{l_i} \exp(i\delta_{l_i}^{+}) \frac{\eta_{l_i}^{\pm}(k_i, r_1)}{r_1} P_{l_i}(\cos(\hat{k}_i . \hat{r}_1)). \tag{6}$$

Where l_i is the angular momentum quantum number of the incident electron. The radial part $\eta_{l_i}^{\pm}(k_i . r_1)$ of the wave function of the incident electron satisfies the intergo — differential equation given by Temkin and Lamkin [16] and corrected for the p-wave by Sloan [17]. $\delta_{l_i}^{\pm}$ is the phase shift.

The total cross section for the electron impact ionization in singlet and triplet modes is given by [18].

$$Q^{\pm} = \int d\hat{k}_f \, d\boldsymbol{k}_e (k_f/k_i) |f_{ion}^{\pm}(\boldsymbol{k}_f, \boldsymbol{k}_i)|^2, \tag{7}$$

where, $\boldsymbol{k}_i$, $\boldsymbol{k}_f$ and $\boldsymbol{k}_e$ are the momenta of the incident, the scattered and the ejected electrons respectively. The ionization amplitude $f_{ion}^{\pm}(\boldsymbol{k}_f, \boldsymbol{k}_e)$ is given by

$$f_{ion}^{\pm}(\boldsymbol{k}_f, \boldsymbol{k}_e) = (2\pi)^{-5/2} \langle \chi_{k_f}(Z_f, \boldsymbol{r}_1) \chi_{k_e}(Z_e, \boldsymbol{r}_2) | V(r_1, r_2) | \psi_i^{\pm}(\boldsymbol{r}_1, \boldsymbol{r}_2) \rangle \tag{8}$$

$\chi_{k_f}(Z_f, \boldsymbol{r}_1)$ and $\chi_{k_e}(Z_e, \boldsymbol{r}_2)$ are the wave functions of the scattered and the ejected electrons, Z_f and Z_e are the effective charges seen by the scattered and the ejected electrons respectively. Following Campeanu et al. [12] we have assumed the complete screening of the residual proton by the ejected electron, i.e. we have into account $Z_f = 0$ and $Z_e = 1$ in our calculations. The interaction potential is taken in the direct channel and it is given by

$$V(r_1, r_2) = -\frac{1}{r_1} + \frac{1}{r_{12}} \tag{9}$$

From (1) and (8), the ionization amplitude can be written as

$$f^{\pm}_{ion}(\boldsymbol{k}_f, \boldsymbol{k}_e) = f^{\pm}_{D}(\boldsymbol{k}_f, \boldsymbol{k}_e) + f^{\pm}_{PD}(\boldsymbol{k}_f, \boldsymbol{k}_e) \pm f^{\pm}_{E}(\boldsymbol{k}_f, \boldsymbol{k}_e) \pm f^{\pm}_{PE}(\boldsymbol{k}_f, \boldsymbol{k}_e). \quad (10)$$

Where $f^{\pm}_{D}, f^{\pm}_{PD}, f^{\pm}_{E}$ and $f^{\pm}_{PE}$ are the direct, the polarized direct, the exchange and the polarized exchange amplitudes, respectively.

$$f^{\pm}_{D}(\boldsymbol{k}_f, \boldsymbol{k}_e) = (2\pi)^{-5/2} \int \chi^{*}_{k_e}(Z_e, \boldsymbol{r}_2)\chi^{*}_{k_f}(Z_f, \boldsymbol{r}_1) \times \\ \times V(r_1, r_2)F^{\pm}(\boldsymbol{r}_1)\Phi_{1S}(\boldsymbol{r}_2)\,d\boldsymbol{r}_1\,d\boldsymbol{r}_2, \quad (11)$$

$$f^{\pm}_{PD}(\boldsymbol{k}_f, \boldsymbol{k}_e) = (2\pi)^{-5/2} \int \chi^{*}_{k_e}(Z_e, \boldsymbol{r}_2)\chi^{*}_{k_f}(Z_f, \boldsymbol{r}_1) \times \\ \times V(r_1, r_2)F^{\pm}(\boldsymbol{r}_1)\Phi_{d}(\boldsymbol{r}_1, \boldsymbol{r}_2)\,d\boldsymbol{r}_1, d\boldsymbol{r}_2. \quad (12)$$

The exchange scattering amplitudes have been obtained by means of the Peterkop condition of exchange [8]

$$f^{\pm}_{E}(\boldsymbol{k}_f, \boldsymbol{k}_e) = f^{\pm}_{D}(\boldsymbol{k}_e, \boldsymbol{k}_f), \quad (13)$$

$$f^{\pm}_{PE}(\boldsymbol{k}_f, \boldsymbol{k}_e) = f^{\pm}_{PD}(\boldsymbol{k}_e, \boldsymbol{k}_f). \quad (14)$$

Now since $Z_e = 1$, i.e. the ejected electron is represented as a coulomb wave in the field of the resudial proton. The wave function $\chi \boldsymbol{k}_e(Z_e, \boldsymbol{r})$ is decomposed into partial waves as

$$\chi \boldsymbol{k}_e(Z_e, \boldsymbol{r}) = 4\pi \sum_{l_e=0}^{\infty} \sum_{m_e=-l_e}^{l_e} i^{l_e} \frac{G_{l_e}(k_e r)}{k_e r} \times Y_{l_e m_e}(\hat{r}) Y^{*}_{l_e m_e}(\hat{k}_e) \exp[-i\eta_{l_e}] \quad (15)$$

where, $G_{l_e}(k_e r)$ is a regular l_eth order coulomb function and η_{l_e} is the coulomb phase shift [19].

Since we have assumed the complete screening of the scattered electron by the residual proton we have calculated the wave function of the scattered electron in the same way as the wave function of the incident electron [12]. We have carried out the partial wave analysis of $f^{\pm}_{D}, f^{\pm}_{PD}, f^{\pm}_{E}$ and $f^{\pm}_{PE}$. Now the total cross section (TCS) for ionization for an unpolarized beam of electrons is given by

$$Q = \frac{1}{4} Q^{+} + \frac{3}{4} Q^{-}. \quad (16)$$

III. RESULT AND DISCUSSIONS

The integral over k_e in the expression for Q has been evaluated by employing the appropriate Gauss-Legendre quadrature. As a check of our computer programme we have reproduced the phase shifts reported by Sloan [17] and

Table 1

Total cross section (in units of πa_0^2) for ($e^- - H(1s)$) ionization

Energy of the incident electron (eV)	FBA results [9]	BE results [7]	Present results	Experimental results	
				ref. [7]	ref. [6]
20.4	0.64	0.476	0.360	0.36	0.35
30.6	1.11	0.804	0.645	0.60	0.58
40.8	1.19	0.889	0.760	0.69	0.67
54.4	1.14	0.883	0.789	0.72	0.70
68.0	1.05	0.836	0.752	0.71	0.69

the BE results of Rudge and Schwartz [7]. Adequate care has been taken to ensure the convergence of Q with respect to the angular momentum quantum numbers l_i, l_f and l_e of the incident electron, the scattered electron and the ejected electron, respectively. The maximum value of l_e was taken as 5. The maximum value $(l_i)_{max}$ of l_i was varied from $(l_i)_{max} = 8$ for $E = 20.4$ eV to $(l_i)_{max} = 12$ for $E = 68$ eV. l_f was obtained by using the traingle rule involving l_i, l_f and l_e. Higher partial waves have been replaced by BE results [7].

Table 1 presents $e^- - H(1s)$, the total ionization cross sections together with the first Born approximation (FBA) results [9], the BE results [7], the recent experimental results of Shah et al. [6] and the earlier experimental results taken from Rudge and Schwartz [7] who have reported a reasonable interpolation of a number of experimental results [2—5]. Our theoretical results are compared in fig. 1 with both sets of the experimental results [6, 7], the Glauber-Exchange (GE) Calculations of Golden and McGuire [9], the pseudostate calculations of Callaway and Oza [11]. The recent experimental results of Shah et al. are marginally lower than the earlier experimental results. The FBA results are appreciably higher than the measured value. The BE results though lower than the FBA results are even higher than those of the experiments. The GE results [9] are less than those of the experiments below 40 eV but at higher energies they exceed the experimental results. The pseudostate results [11] lie below the experimental results. As evident from figure 1 and also mentioned by Callaway [20], the results of Callaway and Oza [11] are not fully convergent. Callaway [20] suggested a better method of obtaining the ionization cross cection at a single incident energy of 15 eV but his result still is below that of the experiment. It is evident from Fig. 1 and table 1 that the present set of results is in good agreement with the experimental results in comparison with other theoretical results shown in figure 1. Moreover, the present method reacher a broad maximum in the total cross section as found in the experiment and the position of the maximum as predicted by the present method agrees fairly with that of the experiment.

So we find that the present distored wave method can predict total ionization cross sections in fairly good agreement with experimental results as found by Campeanu et al. [12] in the case of the e^- – He ionization.

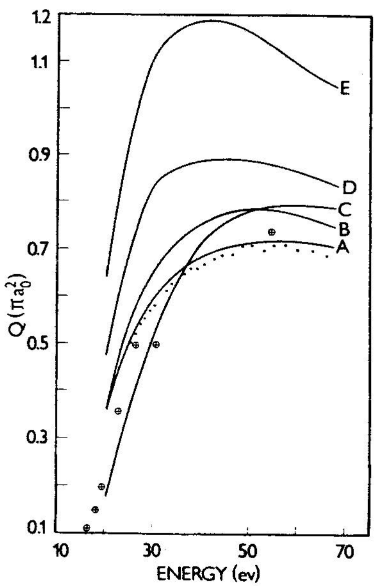

Fig. 1. Total cross section for the electron impact ionization from the ground state of atomic hydrogen (in units of πa_0^2). A: Experimental results [7], B: Present results, C: GE results [9], D: BE results [7], E: FBA results [9], ●: Experimental results [6], ⊕: Pseudostate results [11].

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ПОЛНОЕ СЕЧЕНИЕ [e^- – H(1s)] ИОНИЗАЦИИ

Вычислены полные сечения электронной ударной ионизации основного состояния водорода в диапазоне энергий электронов 20,4 – 68 эВ, методом искаженных волн, где взяты во внимание влияние мишени и скажение в выходном канале. Результаты сравниваются с экспериментальными и теоретическими результатами.