# Ionization of the hydrogen atom from the 2s state by electron impact

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The ionization cross section of hydrogen atom from the metastable 2s state has been calculated in the energy range 5.0—30 eV by using different approximations. The distorted-wave Born approximation has been obtained by solving the static-plus-exchange equation. The present results obtained using the double-Coulomb approximation (in which both the scattered and the ejected electrons are considered to be a Coulomb function with unit charge) are more reliable and are in better agreement with the measured values than other theoretical predictions above 15 eV.

## I. INTRODUCTION

The absolute measurements of the ionization cross sections of hydrogen atoms in the metastable 2s state ($\sigma_{\rm ion}^{2s}$) by electron impact have been reported by three experimental groups (Koller,[1] Dixon, Harrison, and Smith,[2] and Defrance, Clayes, Carnet, and Poulart[3]). Koller[1] first performed the experiment to obtain $\sigma_{\rm ion}^{2s}$ in the energy range 3.4—10 eV. Dixon *et al.*[2] extended the energy range up to 498.5 eV. Recently, Defrance *et al.*[3] have reinvestigated the problem. They have tried to improve the results of earlier experiments and reported the value of $\sigma_{\rm ion}^{2s}$ in the energy range 6.3—998.3 eV. This process has also been studied by a few theoretical workers. Swan[4] has calculated the $\sigma_{\rm ion}^{2s}$ using the first Born approximation (FBA). Burke and Taylor[5] have predicted the $\sigma_{\rm ion}^{2s}$ using the Born (a), Born-Oppenheimer (BO) and three-state close-coupling (3CC) approximations. Rudge and Schwartz[6] have also investigated the problem using the Born (b) and Born-exchange (BE) approximation. Independently, Prasad[7] has also reported the $\sigma_{\rm ion}^{2s}$ using the FBA, BE and Born-Ochkur approximations. All the experimental results are in mutual agreement and lie well below all the theoretical predictions below 40 eV. The situation suggests that this process should further be investigated theoretically in the said energy range.

In our earlier investigation (Ghosh, Majumdar, and Basu[8]) we have calculated the $e^-$-H(1s) ionization cross section ($\sigma_{\rm ion}^{1s}$) using the distorted-wave Born approximation, double-Coulomb approximation (DCA), and its distorted-wave version (the details of the methods are given in Sec. II of the paper). It may be mentioned that the second-order effect is important in predicting the triple differential cross section (Byron, Jr., Joachain, and Piraux[9]). Both the recoil and binary peak can be predicted reliably using a second-order method. On the other hand, DCA predicts the triple differential cross section reliably in the binary region (Ghosh, Majumdar, and Basu[10] and Byron, Jr., Joachain, and Piraux[9]). Due to the involvement of very heavy computational labor, it is not practically possible to calculate the total ionization cross section using the method of Byron *et al.*[9] On the other hand, the total ionization, obtained by using DCA and its distorted-wave version, are in close agreement with the measured values except near the threshold energy. Considering all these facts, we have applied these methods to investigate the present problem.

## II. THEORY

The scattering amplitude for ionization is assumed to be of the form

$$f_{\rm ion}^{\pm}(\mathbf{k}_f,\mathbf{k}_c)=\left\langle \chi_{\mathbf{k}_f}^{*}(Z,\mathbf{r}_1)\chi_{\mathbf{k}_c}^{*}(Z,\mathbf{r}_2)\left|-\frac{1}{r_1}+\frac{1}{r_{12}}\right|\Psi^{\pm}(\mathbf{r}_1,\mathbf{r}_2)\right\rangle , \tag{1}$$

where

$$\Psi^{\pm}(\mathbf{r}_1,\mathbf{r}_2)=(1\pm P_{12})[\Phi_{2s}(\mathbf{r}_2)F^{\pm}(\mathbf{r}_1)] . \tag{2}$$

Here, $\Phi_{2s}(\mathbf{r}_2)$ is the wave function of the hydrogen atom in the 2s state. $F^{\pm}(\mathbf{r}_1)$ (the superscripts $\pm$ stand for the spin) is

 

the wave function of the incident electron. $\chi_{k_c}(Z,\mathbf{r}_2)$ and $\chi_{k_f}(Z,\mathbf{r}_1)$ are the wave functions of the slower and faster electrons, respectively. In all the models considered here. $\chi_{k_c}(Z,\mathbf{r}_2)$ is a Coulomb wave with unit charge whereas $F^{\pm}(\mathbf{r}_1)$ and $\chi_{k_f}(Z,\mathbf{r}_1)$ are of different forms in different approximations as given below.

*Model DCA.* $\chi_{k_f}(Z,\mathbf{r}_1)$ is the Coulomb function of unit charge and $F^{\pm}(\mathbf{r}_1)=e^{i\mathbf{k}_1\cdot\mathbf{r}_1}$.

*Model DW1.* $\chi_{k_f}(Z,\mathbf{r}_1)$ is the same as in DCA and $F^{\pm}(\mathbf{r}_1)$ satisfies the static exchange equation.

*Model DW2.* $\chi_{k_f}(Z,\mathbf{r}_1)=e^{i\mathbf{k}_f\cdot\mathbf{r}_1}$ and $F^{\pm}(\mathbf{r}_1)$ is the same as in DW1.

The ionization amplitude $f^{\pm}_{\rm ion}(\mathbf{k}_f,\mathbf{k}_c)$ may be written in another form

$$f^{\pm}_{\rm ion}(\mathbf{k}_f,\mathbf{k}_c)=f^{\pm}_d(\mathbf{k}_f,\mathbf{k}_c)\pm f^{\pm}_e(\mathbf{k}_f,\mathbf{k}_c)\ . \tag{3}$$

The direct ionization amplitude $f^{\pm}_d(\mathbf{k}_f,\mathbf{k}_c)$ may be written as

$$f^{\pm}_d(\mathbf{k}_f,\mathbf{k}_c)=\left\langle \chi^{*}_{k_f}(Z,\mathbf{r}_1)\chi^{*}_{k_c}(Z,\mathbf{r}_2)\left|-\frac{1}{r_1}+\frac{1}{r_{12}}\right|\Phi_{2s}(\mathbf{r}_2)F^{\pm}(\mathbf{r}_1)\right\rangle\ . \tag{4}$$

In the case of DW2, we invoke the Peterkop condition of exchange (Peterkop[11])

$$f^{\pm}_e(\mathbf{k}_f,\mathbf{k}_c)=f^{\pm}_d(\mathbf{k}_c,\mathbf{k}_f) \tag{5}$$

to evaluate $f^{\pm}_{\rm ion}(\mathbf{k}_f,\mathbf{k}_c)$. In case of DCA and DW1, this condition is automatically satisfied.

After performing the partial-wave analysis, $f^{\pm}_d(\mathbf{k}_f,\mathbf{k}_c)$ is expressed as (using the same notation as Ghosh *et al.*[8])

$$\begin{aligned} f^{\pm}_d(\mathbf{k}_f,\mathbf{k}_c)=(4\pi)^{5/2}\sum_{l'}\sum_{m}\sum_{\lambda} & i^{l'-L-\lambda}(2l'+1) \\ & \times\left[\frac{2l+1}{2\lambda+1}\right]^{1/2}(-1)^m Y^{*}_{lm}(\hat{\mathbf{k}}_c)Y^{*}_{\lambda\mu}(\hat{\mathbf{k}}_f)C\begin{bmatrix} l & l' & \lambda \\ 0 & 0 & 0\end{bmatrix}C\begin{bmatrix} l & l' & \lambda \\ -m & 0 & -m\end{bmatrix}e^{i(\delta_{l'}+\eta_l+\eta_\lambda)}\frac{1}{2l+1} \\ & \times\int_0^{\alpha}H_\lambda(k_f r_1)\frac{u^{\pm}_{l'}(k_i,r_1)}{r_1}r_1^2dr_1\int_0^{\infty}H_l(k_c r_2)R_{2s}(r_2)\frac{r^{l}_{<}}{r^{l+1}_{>}}r_2^2dr_2\ , \end{aligned} \tag{6}$$

where $u^{\pm}_{l'}(k_i,r_1)$, $H_l(k_c r_2)$, and $H_\lambda(k_f r_1)$ are the corresponding radial parts of $F^{\pm}(\mathbf{r}_1)$, $\chi_{k_c}(Z,\mathbf{r}_2)$, and $\chi_{k_f}(Z,\mathbf{r}_1)$. $R_{2s}(r_2)$ is the radial part of the wave function of the hydrogen atom in the $2s$ state.

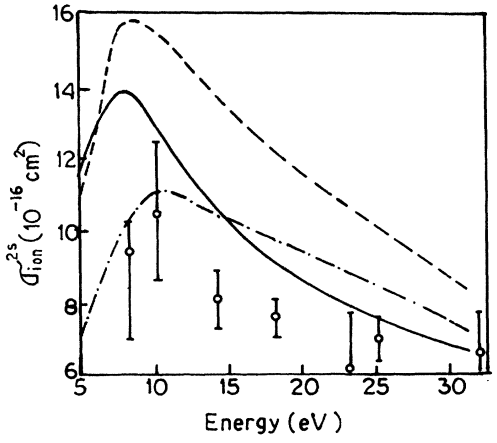


FIG. 1. Ionization cross section of a hydrogen atom from the $2s$ state by electron impact ($\sigma^{2s}_{\rm ion}$) in units of $10^{-16}$ cm$^2$. The curves are the following: ——, present DCA results; — — —, Born-exchange; —·—·—·, BE results of Prasad (1966). The experimental results: Φ, Defrance *et al.* (1981).

## III. RESULTS AND DISCUSSIONS

In calculating the ionization cross section, we have performed the summation up to $l=6$. The summation over other partial waves has been performed until the results for particular $l$ are convergent. The higher partial-wave cross section corresponds nearly to the terms of a geometric series. Therefore, the contributions of partial waves $l>6$ are approximated by the series. It has been verified at the lowest energy that the error incurred due to this approximation is less than 1%.

Figure 1 represents the present DCA result. In the present scale of the figure, the DW1 results cannot be distinguished from the DCA results. Figure 1 also contains BE results, those of Prasad[7] along with the measured values of Defrance *et al.*[3] As in the case of a ground-state hydrogen atom (Ghosh *et al.*[8]), present results are not in good agreement with the measured values near the threshold energies. Above 15 eV, our DCA results are found to

TABLE I. $\sigma^{2s}_{\rm ion}$ ($\pi a_0^2/16$) in different approximations.

| Energy (eV) | $\sigma^{2s}_{\rm ion}$ BE | DW2 | DCA | DW1 |
|---|---|---|---|---|
| 5.1 | 0.75 | 0.78 | 0.85 | 1.11 |
| 7.65 | 1.12 | 1.14 | 0.99 | 1.07 |
| 10.2 | 1.11 | 1.13 | 0.89 | 0.94 |
| 13.6 | 1.00 | 0.97 | 0.80 | 0.83 |
| 17.0 | 0.89 | 0.89 | 0.68 | 0.70 |

be meaningful and are in the best agreement with the measured values among all other theoretical predictions. As in the case of $e^-$-$H(1s)$ ionization (Ghosh *et al.*[8]) the effect of distortion of the incident channel (Table I) influences the results rather marginally. The cross sections are found to be sensitive to the final channel wave functions. The use of DCA near the threshold energy is not very encouraging.

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