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Theoretical Study of Atomic Excitation by Impact of Protons in the Variational Formalism

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Schwinger's variational principle is used to evaluate excitation cross-sections of hydrogen atom by proton impact in a range of energies excluding a pertubative treatment. To describe the strong coupling between the excitation and the capture channels that exists at low energies, the continuum states have been introduced in the total wave function. Our results show that these states can describe properly the projectile capture states.

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1. Introduction

The aim of our study is to appreciate the contribution of the continuum states of the target at intermediate energies in the calculation of total cross-sections of hydrogen atom excitation by proton impact. The continuum states are described by exact wave functions represented as confluent hypergeometric functions. Nevertheless, we should like to mention that to evaluate the variational transition amplitude, two matrix elements types must be calculated: Born I and Born II matrix elements.

In the present work, we are interested in the excitation of the hydrogen atom by proton impact with energies ranging from 2 keV to 200 keV. Our obtained results are compared to other theoretical and experimental results.

2. Theory

To evaluate the variational transition matrix, we use the eikonal method developed by Glauber [1]. In this semiclassical approach, the nuclei are assumed to be moving in a classical manner, while the movement of electrons is described by quantum equations. The initial and final scattering states $|\psi_\alpha^+(z)\rangle$ and $\left|\psi_\beta^-(z)\right\rangle$, respectively, are solutions of the Schrödinger equation given in the eikonal approximation by

$$\left(-\mathrm{i}v\frac{\partial}{\partial z}+H_\mathrm{T}+V\right)\left|\psi_\chi^\pm(z)\right\rangle=0,\quad (\chi=\alpha \mathrm{or} \beta)\,, \tag{1}$$

where z is the coordinate along the almost straight trajectory of the projectile, V is the interaction energy and H_T is the Hamiltonian of the target. The solution of Eq. (1) can be determined by the following Lippmann–Schwinger equations [2]:

$$\left|\psi_\chi^\pm(z)\right\rangle=|\chi(z)\rangle+\int_{-\infty}^{+\infty}\mathrm{d}z' G_\mathrm{T}^\pm(z-z')V(z')\left|\psi_\chi^\pm(z')\right\rangle, \tag{2}$$

where $|\chi\rangle$ is the solution of the homogeneous equation and $G_\mathrm{T}^\pm$ is the Green operator. The elements of the total cross-section for the excitation process are defined by the relation:

$$\sigma_{\alpha\beta}=2\pi\int_0^{+\infty}\mathrm{d}\rho\rho\left|a_{\alpha\beta}\left(\boldsymbol{\rho}\right)\right|^2, \tag{3}$$

where $\boldsymbol{\rho}$ is the impact parameter and $a_{\alpha\beta}\left(\boldsymbol{\rho}\right)$ is the transition amplitude defined as follows:

$$a_{\beta\alpha}\left(\boldsymbol{\rho}\right)=\left(-\frac{\mathrm{i}}{v}\right)\left(\psi_\beta^-\left|V\right|\psi_\alpha^+\right). \tag{4}$$

To calculate $a_{\beta\alpha}\left(\boldsymbol{\rho}\right)$, the states $|\psi_\alpha^+\rangle$ and $\left|\psi_\beta^-\right\rangle$ are expanded over truncated basis sets $|i\rangle$ and $|j\rangle$, respectively. The two basis sets are not necessarily identical but they must have the same finite dimension N. Therefore, Eq. (4) takes the following form:

$$a_{\beta\alpha}\left(\boldsymbol{\rho}\right)=\left(-\frac{\mathrm{i}}{v}\right)\sum_{i=1}^{N}\sum_{j=1}^{N}\left(j\left|V\right|i\right), \tag{5}$$

The expansion of the initial and final states over a truncated basis sets provide an approximate solution for the transition amplitude. To improve the accuracy of this latter, we use the fractional form of the Schwinger variational principle given as follows [3]:

$$\left(j\left|V\right|i\right)=\left(\beta\left|V\right|i\right)\left(D^{-1}\right)_{ij}\left(j\left|V\right|\alpha\right), \tag{6}$$

where $\left(D^{-1}\right)_{ij}$ is an element of the inverse of the matrix D defined as:

$$D_{ij}=\left(i\left|V-VG_\mathrm{T}^+V\right|j\right). \tag{7}$$

To calculate the variational amplitude $a_{\beta\alpha}\left(\boldsymbol{\rho}\right)$, we must evaluate two types of matrix elements: the elements $\left(i\left|V\right|j\right)$ and $\left(i\left|VG_\mathrm{T}^+V\right|j\right)$, namely the first and second order Born approximation, respectively. The first order element is defined as:

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$$(i|V|j) = \int_{-\infty}^{+\infty} \mathrm{d}z \exp\left(\mathrm{i}\frac{\varepsilon_i - \varepsilon_j}{v} z\right) W_{ij}(\rho, z), \qquad (8)$$

where ε_i is the energy of the electronic state $|\varphi\rangle$, and the elements W_{ij} are given as follows:

$$W_{ij}(\rho, z) = \int \mathrm{d}r\varphi_i^*(r) V(R, r)\varphi_j(r)$$

bound-bound transition, (9)

$$W_{ic}(\rho, z) = \int \mathrm{d}r\varphi_i^*(r) V(R, r)\varphi_c(r)$$

bound-continuum transition, (10)

$$W_{cc'}(\rho, z) = \int \mathrm{d}r\varphi_c^*(r) V(R, r)\varphi_{c'}(r)$$

continuum-continuum transition. (11)

The second order element $\left(i\left|VG_T^+V\right|j\right)$ is defined as:

$$\left(i\left|VG_T^+V\right|j\right) = \left[\sum + \int\right]_\nu H_{ij}^\nu, \qquad (12)$$

where the term H_{ij}^ν is given by

$$H_{ij}^\nu = \int_{-\infty}^{+\infty} \mathrm{d}z \exp\left(\mathrm{i}\frac{\varepsilon_i - \varepsilon_\nu}{\nu} z\right) W_{i\nu}(\rho, z) \times \int_{-\infty}^{z} \mathrm{d}z' \exp\left(\mathrm{i}\frac{\varepsilon_\nu - \varepsilon_j}{\nu} z'\right) W_{\nu j}(\rho, z'). \qquad (13)$$

3. Results and discussion

Our work is focused on the study of excitation of the hydrogen atom by proton impact for an energy range between 2 keV and 200 keV. Less than 40 keV the excitation and capture channels become competitive. This is why the initial and final states both are developed on a basis consisting of exact wave functions that describe the bound and continuum states. This will improve the accuracy of the cross-section, since the contribution of the continuum states of the target is taken into account.

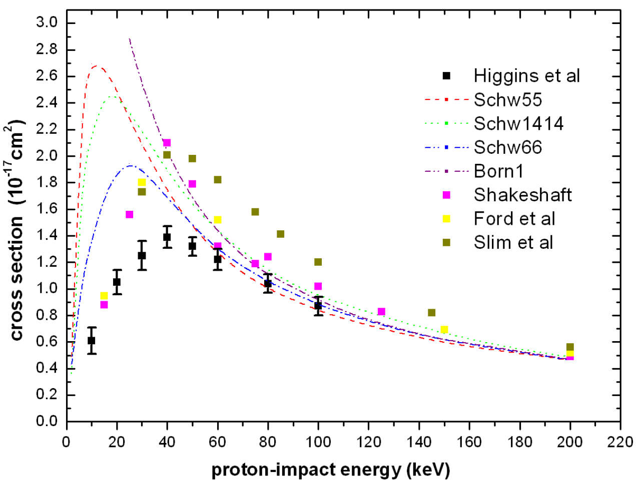

Fig. 1. Total cross-sections for the excitation of the $2s$ state of the hydrogen atom by proton impact.

Figure 1 represents our theoretical results (Schw66) of the total cross-section for the excitation of the $2s$ state of the hydrogen atom by proton impact, compared to experimental results (Higgins et al. [4]) and other theoretical results (Schw55, Schw1414, Born1, Shakeshaft [5], Ford et al. [6] and Slim [7]).

As a first attempt, we have introduced in the initial and final scattering wave functions, a single continuum state of the target with a momentum $k = 0.75$ a.u. The value of k has been obtained thanks to the work of Sahlaoui and Bouamoud [8], DalCappello et al. [9] and Benmansour et al. [10]. Our calculations have therefore been made on an expansion over the finite basis vectors $|i\rangle$ and $|j\rangle$ consisting of the six states $\{1s, 2s, 2p_0, 2p_{+1}, 2p_{-1}, kp_0\}$. The results of our variational method are called Schw66 (Schw as Schwinger and 66 refer to six states in both initial and final states).

From Fig. 1 we can see the good agreement between the present results and those obtained by Bouamoud [11]. We can notice also the significant improvement given by our result Schw66 for energies below 40 keV, compared to the previous results Schw55 and Schw1414 of Bouamoud [11]. For energies above 40 keV, the curves have the same profile.

4. Conclusion

In conclusion, we note that the continuum states of the target are able to properly describe the capture states of the projectile in an energy range where the coupling between capture and excitation channels is very strong.

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