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# ANGULAR-DIFFERENTIAL CROSS SECTION FOR SINGLE ELECTRON CAPTURE TO $H(2p)$ IN PROTON-HELIUM COLLISIONS

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**Abstract:** In this paper we reported new theoretical data using the first Born approximation with correct boundary condition (CB1)[1] for angular differential cross section for $H(2p)$ formation in proton-helium collisions at incident energy 100 keV in the range of scattering angle between 0 and 1 *mrad*. The agreement between the theoretical results and the most recent experimental data is satisfactory.

## 1. Introduction

Single electron capture from multielectron atoms has been studied over many years due to the importance of charge-transfer cross-sections in various applications, particularly in diagnostics of fusion plasmas. Namely, charge exchange recombination spectroscopy is standard technique in high-temperature plasma diagnostics. Electron transfer in ion-atom collision leads to a new atomic system which is formed preferentially in its excited states. The decay of excited states generates radiation losses which can be estimated if the state-to-state capture cross section are known. Computations of the differential cross section for capture into individual hydrogenic $H(2p)$ state are carried out by the first Born approximation with correct boundary condition (CB1 approximation). CB1 theory for electron capture from an arbitrary initial to an arbitrary final state is originally formulated by Belkić *et al* [1]. This approximation was systematically tested on a lot of collision processes (see for example [2,3,4]). Generally, we can say that results of CB1 approximation for the total cross sections are in a good agreement with experimental data at high and intermediate energies. Of course, the differential cross section is more rigorous test of validity of some theory than the total cross section. CB1 approximation, so far applied in Ref.5 for calculation of the differential cross section for the electron capture by proton from K-shell of $H$ and $Ar$. Recently, Seely *et al* [8] reported experimental data for angular differential cross section for $H(2p)$ formation in proton-helium collisions at proton energy 20, 50 and 100 keV. They made measurements by time-correlating hydrogen atoms emerging from collision region with photons emitted perpendicular to scattering plane. These were the first state-selected measurements of angular-differential cross section in this energy range.

Atomic units will be used throughout unless otherwise stated.

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## 2. Theory

In this work the angular-differention cross-sections are studied for the following process:

$$H^+ + He(1s^2) \rightarrow H(2p,\theta) + He^+(1s) \tag{1}$$

where $\theta$ is the scattering angle. We shall use the Roothan-Hartree-Fock (RHF) model [3]. In this model, the initial target state is described by a linear combination of the normalized Slater type orbitals with the parameters obtained by Clementi and Roetti [6]. Wave function of Clementi and Roetti has analytical form for target atom $He(^1S)$:

$$\begin{aligned}\varphi(r) =& 0.76838\exp(-1.41714\,r) + 0.22346\exp(-2.37682\,r) + 0.04082\exp(-4.39628\,r) - \\ & 0.00994\exp(-6.52699\,r) + 0.00230\exp(-7.94252\,r).\end{aligned} \tag{2}$$

The 'active' electron, moves in the field of the effective charge [1]: $Z_T^{eff} = \sqrt{-2\epsilon_i} = 1.354954$, where $\epsilon_i$ is the RHF orbital energy obtained variationally [6] with $\epsilon_i = -0.91795$. The 'passive' electron occupy the same orbital before and after the collision. The 'prior' form transition amplitude $T_{if}(\vec{\eta})$ in the CB1 approximation is given in the following form [1]:

$$T_{if}(\vec{\eta}) = \mathcal{F}\iint d\vec{R}d\vec{r}_T\varphi_f^*(\vec{r}_P)\left(\frac{Z_P}{R} - \frac{Z_P}{r_P}\right)\varphi_i(\vec{r}_T)\exp(i\vec{\alpha}\cdot\vec{r}_T + i\vec{\beta}\cdot\vec{r}_P + i\xi\ln(vR - \vec{v}\cdot\vec{R})), \tag{3}$$

with

$$\mathcal{F} = (\rho v)^{2iZ_T^{eff}(Z_P-1)/v}, \qquad \xi = \frac{Z_T^{eff} - Z_P}{v} \tag{4a}$$

$$\vec{\alpha}\cdot\vec{r}_T + \vec{\beta}\cdot\vec{r}_P = \vec{k}_i\cdot\vec{r}_i + \vec{k}_f\cdot\vec{r}_f \tag{4b}$$

where $Z_P$ is the nuclear charge of the projectile, $\vec{r}_T(\vec{r}_P)$ - position vector of the electron relative to $Z_T(Z_P)$, $\rho$ is the impact parameter, $\varphi_i(\vec{r}_T)$, $\vec{k}_i$ and $\vec{k}_f$ are the initial and final momenta, $\vec{r}_i(\vec{r}_f)$ is position vector of the center of mass of system $Z_T - e(Z_P - e)$ relative to $Z_P(Z_T)$, respectively. Further, $\varphi_f(\vec{r}_P)$ are initial and final bound state wave functions with appropriate energies $\epsilon_i$ and $\epsilon_f$, $\vec{\eta}$ is the transverse momentum transfer $\vec{\eta} = (\eta\cos\phi_\eta, \eta\sin\phi_\eta, 0)$, $\vec{v}$ is the vector of incident velocity. Vectors $\vec{\alpha}$ and $\vec{\beta}$ defined in following way:

$$\vec{\alpha} = \vec{\eta} + \left(\frac{\Delta\epsilon}{v} - \frac{v}{2}\right)\hat{\vec{v}}, \qquad \vec{\beta} = -\vec{\eta} - \left(\frac{\Delta\epsilon}{v} + \frac{v}{2}\right)\hat{\vec{v}}, \qquad \Delta\epsilon = \epsilon_i - \epsilon_f,$$

where $\hat{\vec{v}} = (0,0,1)$ and $\vec{\alpha}+\vec{\beta} = -\vec{v}$. In our case the projectile charge is $Z_p = 1$, which implies that phase factor $\mathcal{F} = 1$, and consequently the differential cross section is proportional to $|T_{if}(\vec{\eta})|^2$.

Six dimensional integral in Eq.(3) can be reduced [1] to one dimensional integral which is evaluated numerically by Gauss-Legendre quadrature.

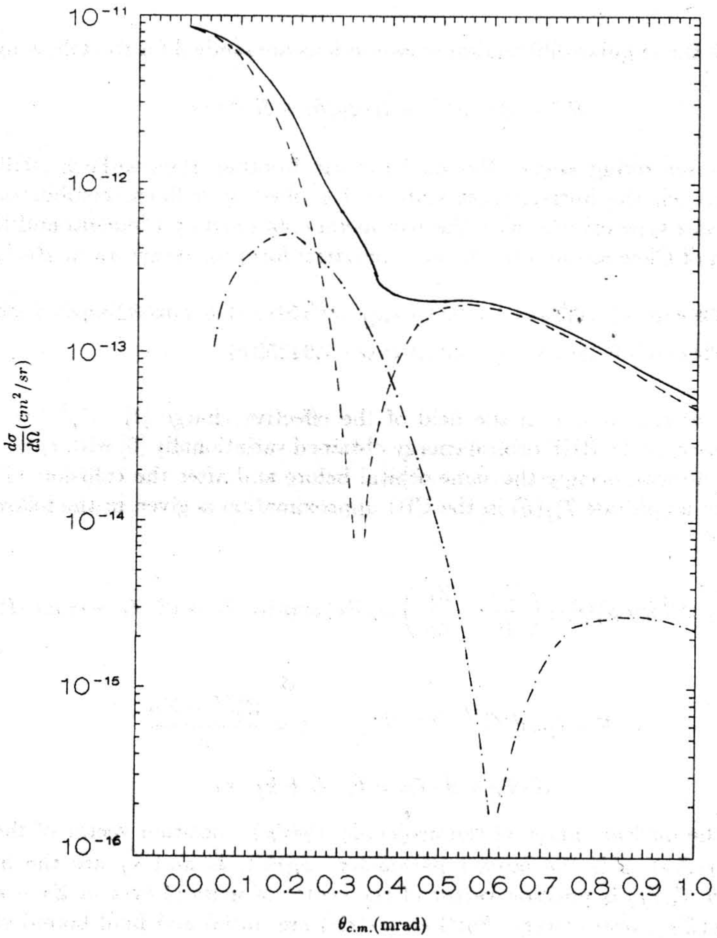


**FIGURE 1** *Differential cross sections for process (1) (see text) at an impact energy of 100 keV. The dashed line is the result of capture into $n = 2, l = 1, m = 0$ state, whereas the dash-dot-dash line refers to state $n = 2, l = 1, m = 1$. The solid line represent the cross section for capture into the 2p state of $H(2p)$..*

## 3. Results and Discussions

General programme of Belkić [7] is applied to calculate the differential cross section for $H(2p)$ at the incident energy of $100 keV$ and center-of-mass scattering angles between 0 and 1 *mrad*.

Differential cross section for $2p$ state is obtained from the following equation:

$$\left(\frac{d\sigma}{d\Omega}\right)_{2p} = \left(\frac{d\sigma}{d\Omega}\right)_{m=0} + 2\left(\frac{d\sigma}{d\Omega}\right)_{m=1}.$$

Unlike the experimental work [8] where the partially contributions to differential cross

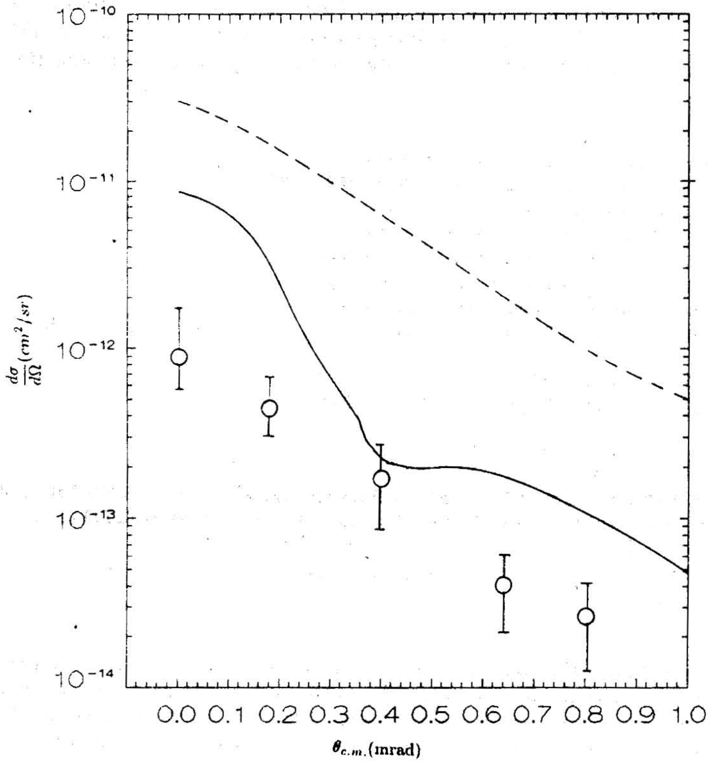


FIGURE 2 *Differential cross sections for process (1) at an impact energy of* 100 $keV$. *The solid line shows present results. The dashed line is CBK approximation [9]. Experimental data: Seely et al [8]..*

section from $m = 0$ and $m = \pm 1$ are not separated, in this papers on Fig. 1 we present state selected angular differential cross sections. In the CB1 approximation differential cross section shows unphysical narrow dips at $\simeq 0.36\,mrad$ for $m = 0$ and $\simeq 0.61\,mrad$ for $m \pm 1$. On Fig.2 is plotted differential cross section for reaction (1). The present results are compared with experimental data recently reported by Seely *et al* [8] and with Coulomb-Brinkman-Kramers (CBK) approximation results [9]. It can be concluded that the theoretical data of CB1 approximation using RHF model are in better agreement with experimental data then CBK approximation. CB1 model is a high-energy approximation and we have compared with experimental measurements only theoretical data for incident energy at $E = 100\,keV$, because at the other energies ($E = 20\,keV$ and $E = 50\,keV$ agreement with experiment is worse. In future some approximation second order should be tested on the reaction (1) for examples: Continuum Distorted Wave approximation (CDW), Boundary Corrected Continuum Distorted Wave (BCIS), Second Born approximation with correct boundary condition (CB2). State selected total cross section at incident energy $100\,keV$ in CB1 approximation are $\sigma_{210} = 1.06[-18]\,cm^2$,

$\sigma_{211} = 1.62[-19]\,cm^2$ and $\sigma_{2p} = \sigma_{210} + 2\sigma_{211} = 1.38[-18]\,cm^2$. Total cross section is given by relation $\sigma_t = \sigma_{1s} + 1.61(\sigma_{2s} + \sigma_{2p})$ . At energy 100 $keV$ we have $\sigma_t = 2.68[-17]\,cm^2$ which is in excellent agreement with the experimental datum given by Barnett and Reynolds [10].

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## DIFERENCIJALNI EFIKASNI PRESEK ZA ZAHVAT ELEKTRONA U $H(2p)$ PRI SUDARU PROTONA SA ATOMOM HELIJUMA

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**Sadržaj:** U ovom radu saopštavamo nove teoriske podatke, dobijene korišćenjem prve Bornove aproksimacije sa korektnim graničnim uslovima (CB1)[1] , zadiferencijalni efikasni presek formiranja $H(2p)$ u sudaru protona sa atomom helijuma pri upadnoj energiji 100 $keV$ u oblasti uglova između 0 i 1 $mrad$. Slaganje naših rezultata sa najnovijim eksperimentalnim rezultatima zadovoljavajuće je.