FULLY DIFFERENTIAL CROSS SECTIONS
OF PROTON-HYDROGEN AND ANTIPROTON- HYDROGEN COLLISIONS

G. ZORIGT*, L. KHENMEDEKH AND CH. ALDARMAA

Department of Physics,
School of Applied Sciences, Mongolian University of Science and Technology.

ABSTRACT

Nonrelativistic collision of proton and antiproton with hydrogen atom described by solving time-dependent Schrodinger equation numerically. Coulomb wave function discrete variable method (CWDVR) had been used to calculate electron wave function evolution, while projectile defined classically, moving along the straight line trajectories with constant velocity. The ionization amplitude calculated by projection of the wave function into continuum wave function of the hydrogen electron. The fully differential cross sections calculated depending on projectile impact energy, scattering angle and electron ejection energy and angles. Our results in good agreement with the relativistic calculation results.

1. INTRODUCTION

Theory of charged particle collision had been studied from establishment of quantum theory in the middle of 1920s, beginning from the Born theory of collision. Experimental equipment's are continuously improved, and can accurately measure the differential cross sections of the collision. From the computational point of view, the antiproton collision with Hydrogen atom is simplest case, because against the proton case, the electron capture channel doesn't contribute to the collision cross section.

In the resent years, few theoretical works among them perturbative theory of Voitkiv *et al.* [1] based on Continuum Distorted Wave (CDW) approximation. At low energy of projectile, for few hundred keV, the perturbation theory become inaccurate, and non perturbative theory can be applied. Recently, developed few non preturbative theories, treating the projectile classically, as moving along a straight line, but the atomic electrons treated quantum mechanically. Among them, coupler pseudo state (CP) theory of McGovern *et al.* [2,3], time dependent convergent – close – coupling (QM - CCC) approach (Abdurakhmanov *et al.* [4]) , time dependent close coupling (TDCC) method (Ciappina *et al.* [5]) could be mentioned. Recently, Boudarev *et al.* [6] used the relativistic single center semi classical coupled channel approach had been developed to calculate fully differential cross section (FDCS).

In the present study, for the first time, the Coulomb wave functions have been used as a basis in the discrete variable representation (L.Y. Peng, A.F Starace [7]) to study the antiproton-hydrogen collisions. These wave functions have been first expanded into the spherical harmonic functions as they enable to explicitly calculate the time-dependent radial functions. By considering the classical assumption that an antiproton with a particular impact parameter preserves its straight trajectory, we show how the hydrogen electron has temporally evolved from its ground state in the field produced by the presence of the antiproton and compared the results of the FDCS to the previously published theoretical data. In particular, we compare our results for the FDCS-s in the antiproton and proton -atom collision, in which an initially 200 – 900 keV energetic antiproton is momentum transfer 0.1 au. to the previously published results.

2. THEORY

Assuming the antiproton moving along the straight trajectory, the atomic electron excitation and/or ionization processes are studied here as functions of the antiproton impact parameter. We adopt numerical approach constructing a space net and calculate the wave function on each knot of the net in the spherical coordinate system. This is accomplished by solving the one of the fundamental equations of the quantum mechanics – the time-dependent Schrödinger equation. Namely, the Schrödinger equation for an electron of the hydrogen atom in the external field is given by

$$i\frac{\partial \Psi(\vec{r},t)}{\partial t} = \left(\widehat{H}_0 + \widehat{V}(\vec{r},t) \right) \Psi(\vec{r},t) \tag{1}$$

Corresponding Author: G. Zorigt*

where $\Psi(\vec{r}, t)$ is wave function and $\widehat{H}_0$ is the Hamiltonian for an electron of a hydrogen atom, $\widehat{V}(\vec{r}, t)$ is the interaction opreator due to the external field. Assuming that the antiproton or ion moves along the straight line (z-axis), the produced electric potential is expressed as follows

$$\widehat{V}(\boldsymbol{r}, t) = -\frac{1}{|\boldsymbol{R}(b, 0, vt) - \boldsymbol{r}|} \tag{2}$$

here $\boldsymbol{R}$ is ion radius vector, b is impact parameter, v is ion velocity, $\boldsymbol{r}$ is electron radius vector, t is time. With this assumption that the antiproton moves along the classical trajectory, the ionization and scattering calculations have been performed in the cases of antiproton-helium [8-10] and antiproton-hydrogen [3-6] collisions. The total differential cross section is the one of the experimentally verifiable quantities as results of ionization processes. Coulomb wave function discrete variable method (CWDVR) had been used to calculate electron wave function evolution, while projectile defined classically, moving along the straight line trajectories with constant velocity.

The ionization amplitude is obtained by an overlap integral constructed from the wave functions calculated in the discrete variable representation as

$$T(\varepsilon, \theta_e, \varphi_e, b, \varphi_b) = \langle \psi^- | \Psi(\vec{r}, t) \rangle \tag{3}$$

where for impact parameter $\vec{b}(b, \varphi_b)$, an electron ionization amplitude for scattering angle θ_e, φ_e and energy ε is $T(\varepsilon, \theta_e, \varphi_e, b, \varphi_b)$ and ψ^- is continuum wave function, $\Psi(\vec{r}, t)$ is wave function at a final moment in the calculation.

Next, the ionization amplitude is converted from its impact parameter representation to the momentum transport representation by two-dimensional Fourier transform as in Bondarev *et al*. [3].
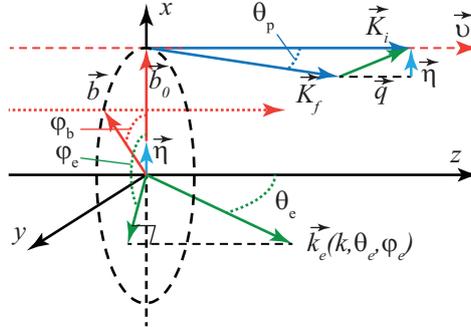

Figure-1: *Antiproton enters along z-axis. $\vec{K}_i, \vec{K}_f$ are initial and final momenta of the antiproton $\vec{k}_e$ is the electron momentum, $\vec{\eta}$ is the component perpendicular to the antiproton velocity $\vec{v}$ of the momentum transport from the antiproton to the atom. θ_p is the antiproton's scattering angle.*

The geometric construction of the vectors for impact parameter and momentum transport is illustrated schematically in Fig. 1. As shown in figure 1, the ionization amplitude is obtained by the integral given in Eq. (4) in the representation of $\vec{\eta}$ - the perpendicular component of the momentum transfer to the antiproton's velocity $\vec{v}$ as follows,

$$T(\varepsilon, \theta_e, \varphi_e, \eta, \varphi_\eta) = \frac{1}{2\pi} \int d\vec{b} e^{i\vec{\eta}\vec{b}} e^{i\delta(b)} T(\varepsilon, \theta_e, \varphi_e, b, \varphi_b) \tag{4}$$

here $\delta(b)$ is the phase shift accounting the ion-atom interaction as given by

$$\delta(b) = \frac{2Z_P Z_T}{v} \ln(vb) \tag{5}$$

Due to the momentum transfer $\vec{\eta}(\eta, \varphi_\eta)$ from the antiproton, assume that the electron is ionized with an energy of ε with angle θ_e, φ_e. The corresponding ionization fully differential cross section is expressed as

$$\frac{d^3\sigma}{d\varepsilon d\Omega_e d\Omega_P} = K_i K_f |T(\varepsilon, \theta_e, \varphi_e, \eta, \varphi_\eta)|^2 \tag{6}$$

where $d\Omega_p$ is differentiation of the scattering solid angle for the antiproton, K_i, K_f are initial and final momenta of the antiproton. In the relative coordinate system, the atomic nucleus is assumed to be at rest and antiproton is expressed with its reduced mass.

3. RESULTS AND DISCUSSION

We consider the proton and antiproton collision with Hydrogen atom in it is ground state. First, we calculated the ionization amplitude for projectile flying along straight-line trajectory with constant velocity and for given impact parameter. Impact parameter b varies with in the integral (0.01-100 a.u.). We used symmetry properties (axial symmetry around the Z- axis, which is parallel to projectile trajectory and mirror symmetry with respect to the scattering plane.) to economy the calculations. The ionization amplitudes for different impact parameters are collected as a data for further calculations of scattering amplitude with given projectile scattering angle using formula (4), in which the integrals calculated numerically.

Then fully differential cross sections are obtained via the formula (6). We perform calculations for different projectile energies and different scattering angles. Fig. 2 shows differential cross sections of ionization for projectile with energy of 200 keV and scattering angle of 0.2 mrad, where electron ejection energy is equal to 4 eV and 10 eV. As it seen from the Fig. 2, our calculations are in agreement with the relativistic cross sections of Bondarev *et al* [6]. At this impact energy, the first Born cross section binary peak is much higher in comparison with our calculated result, but the recoil peak is much smaller.
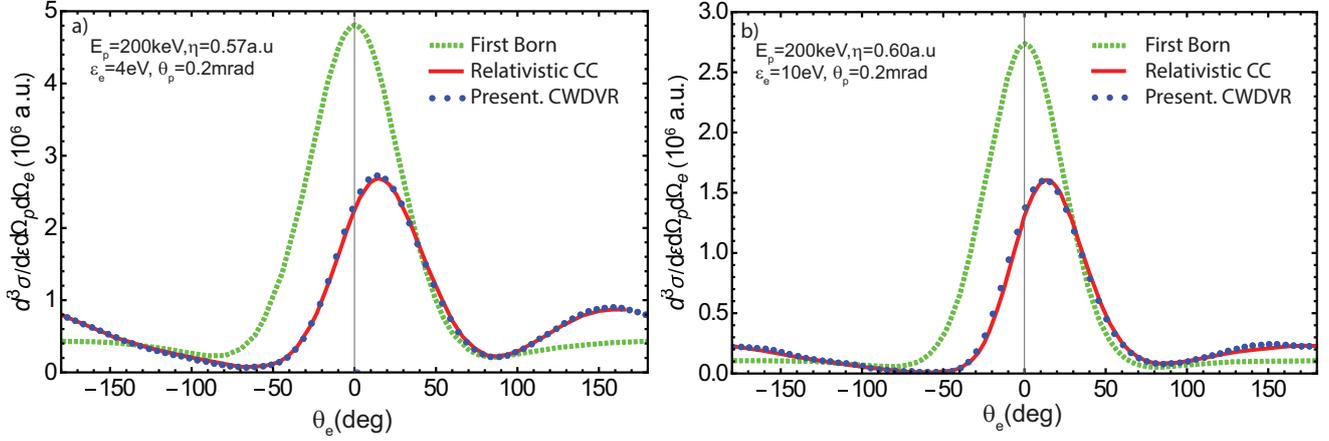

Figure-2: FDCS in the scattering plane. The collision parameters: The projectile energy of 200keV and scattering angle of 0.2mrad, where electron ejection energy is equal to a). 4 eV and b).10eV .The results of the relativistic coupled-channel are from Ref.[6]

Notable shift of the binary and recoil peak direction relative to the first Born peak directions also observed. At the 500keV energy differences between numerical results and first Born approximation has same feature as in the previous energy but getting smaller. Fig. 3.
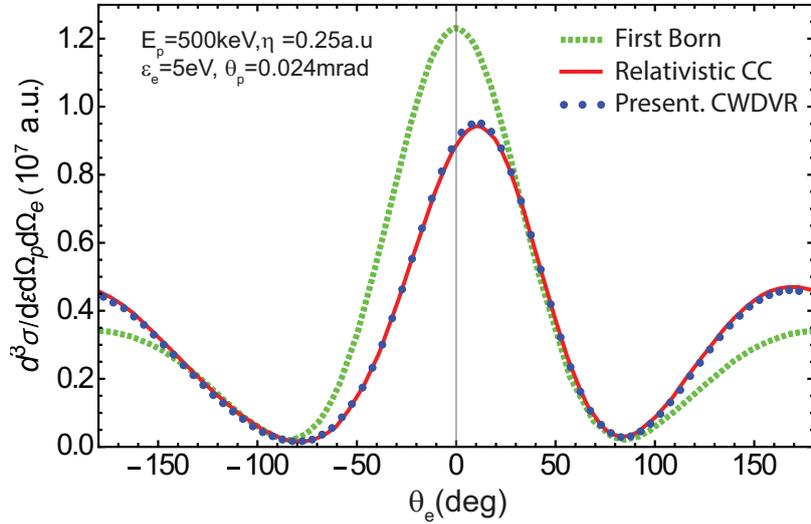

Figure-3: FDCS in the scattering plane.The collision parameters:The projectile energy of 500keV and scattering angle of 0.024mrad, where electron ejection energy is equal to 5eV .The results of the relativistic coupled-channel are from Ref.[6].

Next, we compare our proton and antiproton impact ionization results with CDW cross sections Voitikiv *et.al* [1]. In this case, the binary and recoil peak height and shift for proton are opposite in comparison to the antiproton case, the first Born results lie between proton and antiproton cases. This is of course, the projectile charge effect; first Born approximation does not defend on projectile charge. On the other hand, CDW approximation can handle with charge sign difference, as seen from Fig. 4 but did not fully take into account in comparison to the numerical solution of the Schrödinger equation. At the highest projectile energy of 900keV the CDW cross sections are nearly coincide with numerical cross sections as seen from Fig. 4c.
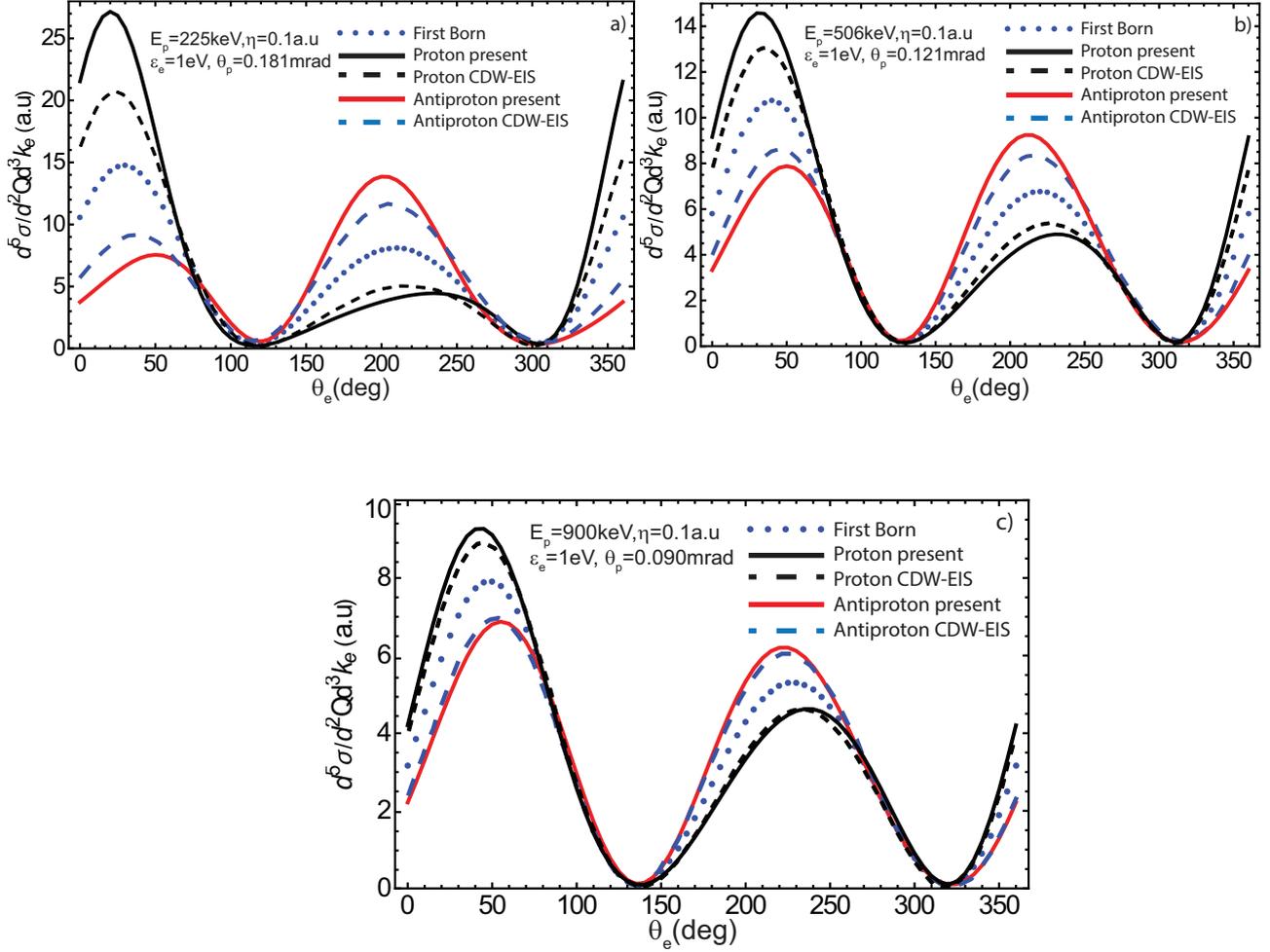
Figure-4: *FDCS in the scattering plane. The collision parameters:The electron ejection energy 1eV and the component perpendicular to the antiproton velocity of the momentum transport 0.1 a. u., projectile energy where is equal to a). 225 keV and b).506 keV c). 900 keV.The results of the CDW from Ref. [1].*

4. CONCLUSIONS

Fully differential ionization cross sections of proton and antiproton collisions with Hydrogen atom are obtained from the numerical solutions of the time dependent Schrödinger equation using CWDVR method.

The calculated FDCS-s are agree will with the relativistic FDCS of Bondarev *et al.* [3]. We test our numerical method for different incident energiys and scattering angles of the projectile and get convergence to the relativistic cross sections Bondarev *et al.*

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