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Ionization of atoms by charged particles

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Abstract. Ionization of hydrogen atom by charged particle impact are studied at different collisional energies and the total and differential cross sections are calculated. In case of light particle impact the final-state wave function here considers all three two-body interactions on an equal footing and satisfies the exact Coulomb boundary conditions. The spin asymmetries are also found and the values are compared with other existing results. For heavy particle impact a final continuum state wave function which incorporates distortion due to the Coulomb fields of both the projectile and the target nuclei is employed. In this case the target hydrogen atom is considered in its ground as well as metastable 2*s* state. The results thus obtained are compared with the existing experimental findings as well as other theoretical predictions.

Keywords. Ionization; positron; antiproton; cross section.

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1. Introduction

Ionization is a well known process that plays a vital role in understanding many astrophysical and plasma phenomena, in particular a knowledge of ionization cross sections for atomic system is essential in the development of fusion research and technology. To date, a good number of theoretical and experimental investigations have been made on the ionization processes. In this article, we discuss the ionization of hydrogen atoms be charged particle impact. Regarding theoretical investigations, hydrogen is the only atomic system for which the initial and final state wave functions are exactly known, so the total ionization cross sections can be evaluated very accurately. We have calculated the ionization probabilities and then cross-sections of atomic hydrogen by electron, positron, proton and anti-proton impact.

The theoretical investigation of the ionization process involves full complexities of the quantum mechanical three body problem and as such is too difficult to solve exactly. We consider here the ionization of atomic hydrogen by electron, positron, proton and anti-proton impact and discuss those in the consecutive sections.

2. Electron impact ionization

Development of the quantum theory of ionization by electron impact may be distinguished into three successive phases.

In 1930s Bethe [1] and Massey and Mohr [2] used the first Born approximation to calculate the ionization cross section of hydrogen atom by electron impact.

The second phase occured during the 1960s when Peterkop [3] and Rudge and Seaton [4] developed theoretical formulations of the problem. They considered the special features due to the presence of three charged particles in the final state. It was still restricted to first order treatments in the electron target interaction though important conceptual progress was made during this second phase of calculation. At that time only the experimental values of total cross sections were available which can not provide a stringent test of the theories. Significant discrepancies between these measurements and first order theories were observed at low and intermediate energies.

The third phase in the development of theories, had been done so far, was stimulated by $(e, 2e)$ coincidence experiments by Ehrhardt *et al* [5] and Amaldi *et al* [6]. Such experiments, in which the kinematics of the collision is fully determined, provided the most complete test of the theory of electron impact ionization reactions. For a long time, several important features of these experiments remained unexplained. At present more refined theoretical investigations have been done with some success and elaborate experimental work for $(e, 2e)$ is being performed at many laboratories. Due to the enormous difficulty, theory is not yet able to give a very satisfactory account of the ionization problem covering the entire energy range. Here the form of the final state wave function, when both the scattered and the emitted electrons are very far from the proton deserves special consideration. To know this, one has to incorporate all the three interactions, the interactions between the scattered electron and the ejected electron as well as interactions between the proton and the scattered electron and the proton and the emitted electron. All these three are long range Coulomb interactions and no one of them should be neglected in comparison with the other two.

Few years back Brauner *et al* [7] gave a form of the scattered wave function for the final state after ionization. This wave function, which depends on three interparticle Coulomb interactions satisfying the asymptotically correct boundary condition involves three appropriate cofluent hypergeometric function as follows:

$$\Psi_f^- = (2\pi)^{-3} \times \exp(ik_a \cdot r_a + ik_b \cdot r_b) \times C(\alpha_{pT}, k_a, r_a) \times C(\alpha_{cT}, k_b, r_b) \times C(\alpha_{eP}, k_{ab}, r_{ab}),$$

where the Coulomb part of the wave function is defined as

$$C(\alpha, k, r) = \Gamma(1 - i\alpha) \exp\left(-\frac{\alpha\pi}{2}\right) \times {}_1F_1(i\alpha; 1; -i(kr + k \cdot r)),$$

where

$$k_{ab} = \tfrac{1}{2}(k_a - k_b), r_{ab} = r_a - r_b.$$

r_a, r_b and k_a, k_b are the position vectors and corresponding momenta of scattered and ejected electrons respectively. Here,

$$\alpha_{\rm PT} = \frac{Z_{\rm P} Z_{\rm T}}{k_a}, \qquad \alpha_{eT} = -\frac{Z_{\rm T}}{k_b}, \qquad \alpha_{eP} = -\frac{\mu_{\rm P} Z_{\rm P}}{k_{ab}}.$$

$Z_{\rm P}$ and $Z_{\rm T}$ are the projectile and target charges and $\mu_{\rm P} = 1/2$.

This asymptotically correct final state wave function has been used with great success by Briggs and co-workers [8a-c], Roy *et al* [9a, b] and Bandyopadhyay *et al* [10a–d] and few others. From the theoretical point of view, calculation of the triple differential cross section (TDCS) is the easiest while the calculations of the double differential (DDCS), single differential (SDCS) and finally the total ionization (TICS) cross sections are increasingly more and more difficult. On the experimental side the situation is just the reverse. In Bandyopadhyay *et al* [10a] we have calculated the TDCS for ionization of hydrogen atom by electron impact including exchange effect using the above correlated three body continuum wave function for the final state.

From the various works on electron impact ionization, it is very clear that the effect of the final state electron–electron correlation is very important in fast electron-atom ionizing collisions, particularly when the relative momentum of out going particles is small. Here all the three two-body interactions should be treated on an equal footing. This has led us to reconsider the investigation of the ionization cross-sections for hydrogen atom by electron impact, employing the symmetric form of the wave function which describes the three-body Coulomb continuum state. We use this wave function to calculate triple, double and single differential cross sections and the total cross sections for investigating the ionization of hydrogen by electron [10a, b, d] and positron [10a–d] impact. In the case of electron impact we have included the exchange effect in our calculations. We compare our triple differential cross section values mainly with the experimental results of McCarthy *et al* [11]. In Ehrhardt asymmetric geometry in which one electron emerges with a high velocity and other one with low velocity, it is observed that the exchange effect is small; but in symmetric geometry, when two electrons emerge with equal velocity, the exchange effect is appreciably high and hence can not be neglected. During our calculation we note that the results including exchange effect are quite sensitive to variation of the absolute value of the relative momentum in the exit channel. Attention is paid to the special case of equal energy sharing in the final channel, where scattered and ejected electron energies are equal and it is found that the exchange effect is remarkably high in this case.

In a separate work [10d], we have also calculated the single differential and total ionization cross sections of a hydrogen atom by electron impact. The calculated values of the single differential cross sections for the energy distribution of secondary electron and the total cross sections are compared with the available theoretical and experimental data. The spin asymmetries are also found and the ionization asymmetry is calculated. The values thus obtained are compared with the existing results.

3. Positron impact ionization

Positron is antiparticle of the electron and bears the same mass but opposite charge. Studies on positron impact ioinization can provide valuable insights into the dynamics of the process since, unlike the situation for electron impact, the projectile positron and the ionized electron are distinguishable. Due to the advancement of techniques within the last few decades the possibility of doing various atomic scattering experiments with positrons has improved much. The point of contact between theories and experiments in scattering problems involving positron have been successfully carried out at many laboratories.

We have computed the results for TDCS, DDCS, SDCS and TICS of hydrogen atom by positron impact for a wide-range of incident energies and scattering parameters [9a, b; 10a–c]. As a projectile, the positron with its positive charge is much unlike the electron and hence significant difference has been observed in the cross sectional values for electron impact and positron impact. We have compared our above mentioned values by positron impact with other existing theoretical and experimental values.

Recently Jones *et al* [12] have measured the total cross sections of ionization of hydrogen atom by electron and positron impact for kinetic energies varying from 15 to 700 eV. Their values for positron impact are found to be significantly lower than those obtained previously by Spicher *et al* [13]. Many theoretical calculations have been done so far for the above and most of the positron impact results are for incident energies below 150 eV. We have calculated the total cross sections of the ionization of hydrogen atom by positron impact for incident energies ranging from 25 to 600 eV and compared them with the available experimental data of Jones *et al* [12] and Spicher *et al* [13]. Our values are in close agreement with the experimental data of Jones *et al* at energies from 75 eV onwards. This shows that the three body Coulomb wave function considered as the final state is quite appropriate for high energies. Other available theoretical values for high energies lie above the values of Jones *et al.*

The cusp-like peak in the energy spectrum of forward ejected electrons emitted in ion-atom collisions was observed in 1970. Many experimental and theoretical works were devoted to clarify the details of this phenomenon. This process is a special case of ionization when ionized electron is strongly influenced by the projectile and their velocities are the same. This process is called the electron capture to the continuum (ECC). The most important mechanism for the appearance of the ECC peak is the focussing of the ejected target electron into the direction of the outgoing projectile, due to the attractive interaction between them.

For positron impact, ECC process has not been discovered experimentally. Only theoretical predictions exist. We [14] were the first who studied positron hydrogen angular scattering and found a pronounced peak in our DDCS results. We used Faddeev three-body wave function. Brauner and Briggs [15a, b] also showed the cusp-like structure at H target.

In a different calculation [10c] of positron-hydrogen ionizing collisions, we predicted pronounced ECC cusps in DDCS. Recently, Finch *et al* [16] performed a measurement to obtain DDCS values for positron–argon collision at 30°. They did not find any evidence for ECC.

4. Threshold law

The energy dependence of the cross section σ for the positron impact ionization of hydrogen atom near threshold is to a large extent determined by the form of final state wave function in quantum mechanical calculations. With one attractive Coulomb function corresponding to full screening of the target nuclear charge; one gets identical results for electron and positron impact in which σ varies as $E^{3/2}$.

With two Coulomb functions, one attractive and the other repulsive, Geltman [17] got an unphysical result for positron impact ionization. For e^+ impact, he got σ as almost insignificant over a considerable portion of the energy interval near threshold. This is due to the normalization constant (for the repulsive interaction) which vanishes exponentially. The phase condition of the final state wave function in the asymptotic region, is satisfied in neither of these two cases of full screening and no screening. Temkin [18] obtained a modulated linear law on the basis of his Coulomb dipole theory.

An asymptotically correct final state wave function which involves three Coulomb functions [19] will involve one repulsive Coulomb function for both e^- and e^+ impact. In the final channel, there will be three interactions: (i) between the projectile and the target nucleus, (ii) between the projectile and the free electron which was originally bound in the atom and (iii) between the free electron and the target nucleus. When the projectile is the electron, the repulsive Coulomb function will correspond to the projectile-electron interaction, and for positron impact on the other hand, the repulsive Coulomb function will correspond to the interaction between the positron and the target nucleus. Therefore according to Brauner *et al* [7] the use of the three Coulomb function in final state for the calculation of ionization cross section near threshold would lead to unphysical results for both electron and positron impact due to the exponential vanishing of the normalization constant arising from the repulsive Coulomb function.

In our recent calculation [19] we have shown how the exponentially vanishing normalization factor due to repulsive positron–proton interaction is appropriately compensated for and a physical threshold law $\sigma \sim E^{3/2}$ is obtained.

For e^- impact ionization, the Wannier [20] model based on classical theory gives a threshold law $\sigma \sim E^{1.127}$ for atomic hydrogen. In general, it is considered to be satisfactory.

Quantum mechansical extension of this model was attempted by Peterkop [21], Rau [22] and others. Klar [23] extended the Wannier model for $e^{\pm}$-impact ionization and obtained analytically a threshold law $\sigma \sim E^{2.65}$ for hydrogen atom.

Kazansky, Ostrovsky and Sergeeva [24] have modified the Wannier threshold law for small but finite energy excess above threshold.

For e^+-impact, the Wannier threshold law is controversial. Dimitrijevic and Grujic [25] have obtained a threshold law $\sigma \sim E^{1.64}$ for e^+-impact on hydrogen, by their classical trajectory study. The CTMC calculations of Wetmore and Olson [26], on the other hand, agree with the power law $\sigma \sim E^{3.01}$.

We have evaluated analytically the cross section σ for e^+-impact ionization of hydrogen atom near threshold with the final state wave function involving three Coulomb functions. In contradiction to earlier result that σ vanishes exponentially we get [19]

$$\sigma = 3^{-1}\pi Z^{12}\exp(-2)(2^{1/2} - 1)E^{3/2}.$$

It may be noted that the Wannier law does not give the absolute magnitude of the cross section, which is required for a quantitative comparison with experiment.

5. Proton and antiproton impact

An accurate knowledge of differential and total ionization cross sections for the collisions of proton with atomic hydrogen has important application in the diagnostics of fusion plasma. Further, the comparative study of ionization of hydrogen atom by antiproton impact has some importance due to the fundamental difference of its charge from proton.

In the case of ionic impact we can simplify the problem by applying the impact parameter formalism in which the projectile ion may be assumed to move in a classical trajectory. However, in the case of ionization the final state contains three charged particles which mutually interact by long range Coulomb forces and as such the theoretical treatment of the problem becomes quite complicated.

Theoretical investigation on ionization by heavy particle collision started with the calculation of the total ionization cross section (TICS) by Bates and Griffing [27] on proton-hydrogen collision by using first Born approximation (FBA). The calculated values in the higher energy region were in good agreement with the experimental data of Gilbody and Ireland [28] who performed their work about ten years later; however, a marked disagreement with the theoretical cross section values were seen below 200 keV with various measured data.

Due to the long range nature of Coulomb potential, the distortion effects are appreciable even when two nuclei are very far apart. Salin [29] used the exact asymptotic condition and considered the distortion of target in the final channel. To improve the agreement with new experimental data for ionization by heavy ions, Crothers and McCann [30] introduced the continuum distorted wave-eikonal initial state (CDW-EIS) model in which the final state was chosen as in CDW, but the initial state was represented by a bound state distorted by projectile eikonal phase.

Initially, only the total ionization cross section (TICS) values for proton impacting on atomic hydrogen were available. Fite *et al* [31], Shah *et al* [32] and Shah and Gilbody [33] measured the TICS values. Recently Kerby *et al* [34] accurately measured the differential cross section in ejected electron energy and angle of ionization of atomic hydrogen and molecular hydrogen by proton impact. As the calculation of TICS involves the interaction momenta of all the three particles in the final state, many important informations regarding the interaction and mechanism of ionization were not clear.

Following the earlier work [35], we propose to apply Born approximation in the impact parameter formalism to calculate the ionization cross section for the collision of hydrogen atom by proton and antiproton impact in the intermediate and high energy region. The final state wave function considers the electron to be moving in the continuum of both the projectile and target nuclei.

Various computed results for the DDCS and TICS for the collision of proton with the ground and $2s$ state of hydrogen atoms are presented and compared with the various existing experimental findings and theoretical calculations. We also present our computed results of the ionization cross section for antiproton as projectile and compare them with the existing theoretical as well as experimental results. Knudsen *et al* [36] have measured the ionization cross sections for antiproton colliding with atomic hydrogen in the energies ranging between 30 to 1000 keV. The experimental results of ionization by antiproton impact has special importance due to the fact that here the absence of electron-transfer channel makes surer test of theoretical methods.

In figure 1, we display our results of the total ionization cross section for collision of proton and antiproton with atomic hydrogen along with the available experimental measurements. The results obtained by classical trajectory Monte Carlo (CTMC) method [37] are also displayed in the figure. For the case of proton impact the present calculated

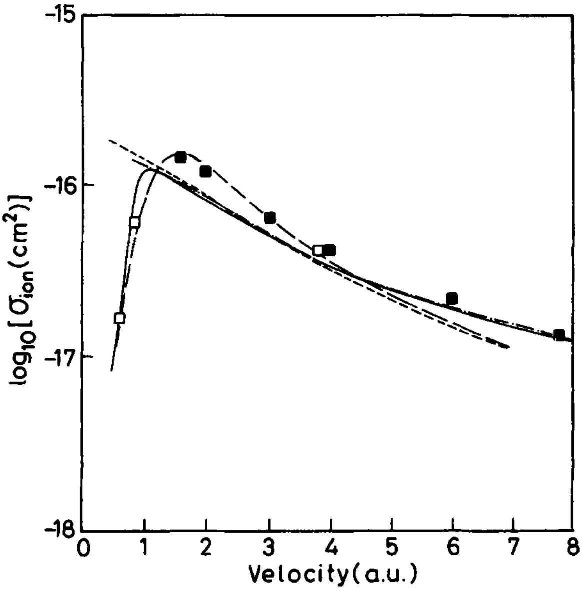

Figure 1. Total cross sections for ionization of atomic hydrogen by proton and anti proton impact. Present results (——) for proton; (–·–·–) for anti proton; CTMC (– – –) for proton, (- - - - - -) for antiproton. Experiment – for proton: □ Shah *et al* [32]; ■ Shah and Gilbody [33].

results are in fairly good agreement with the CTMC results and the experimental measurements [32, 33] throughout the energy region considered. In the case of antiproton the present results almost coincide with CTMC in the low and intermediate energy region. With the increase of energy the present calculated results deviate slightly with the CTMC results.

In figure 2, we compare our values for DDCS as a function of ejection angle with those of CTMC [38], Born [38] and CDW-EIS [38] and the observed data [38]. We have computed our values for ejected electron energy of 130 eV and for 70 keV proton impact. Our results agree well with the experimental data around the ejection angles of 60 to 120 degrees. All the theoretical results including the present one show similar trend with the experimental observation.

In figure 3, we present our results for the total ionization cross sections for $P^- + H(2s)$ and $p + H(2s)$ collisions for incident ion energies of 5 to 100 keV. For comparison we also present the calculated values of Ford *et al* [39] for proton impact obtained by one centered close coupling expansion method. At collision energies above 50 keV the present results for total ionization cross section for $p + H(2s)$ collision agree well with the calculation of Ford *et al* for electron removal cross section, obtained by adding the electron capture cross section with the ionization. From the calculated results it appears that the ionization cross section for collision with H(2*s*) in the case of proton impact are about as high as those obtained by the collision of antiproton. In the same figure we also present the results of Chen *et al* [40] for direct ionization of $p + H(2s)$ collision obtained by two-center atomic orbital close coupling method.

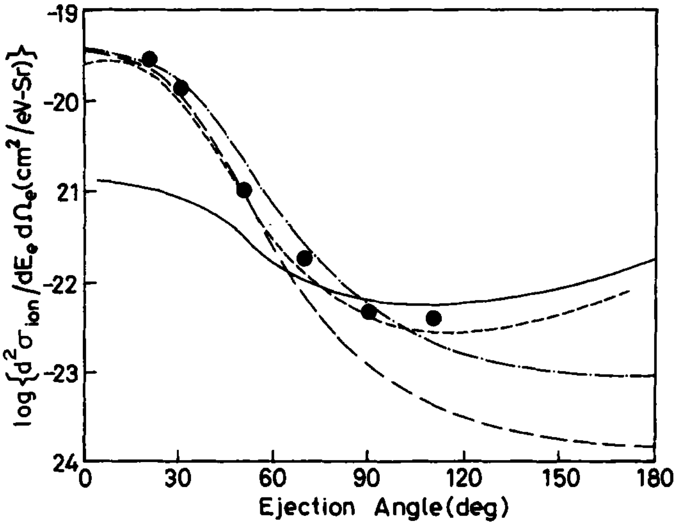

Figure 2. DDCS results for ionization of atomic hydrogen by 70 keV proton impact as a function of ejection angle for ejection energy of 130 eV. Present result (———); CTMC [38] (- - - - - -); CDW-EIS [38] (– – – –); Born [38] (–·–·–); Experiment [38] (•).

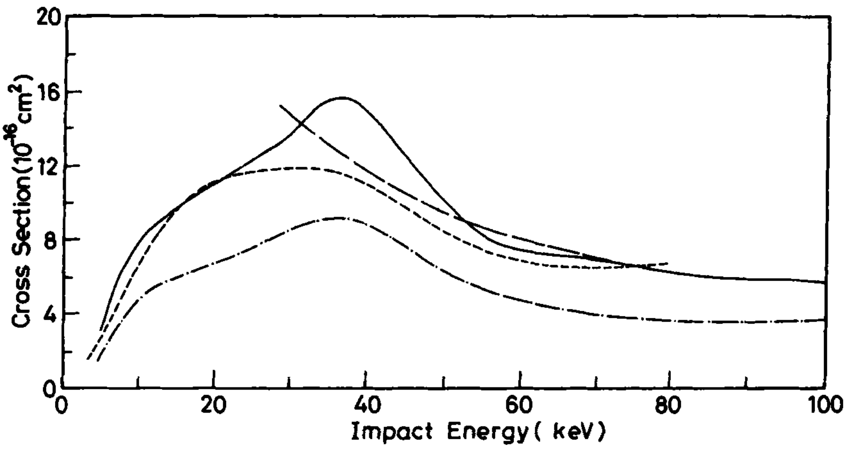

Figure 3. Total cross sections for ionization of H(2s) by proton and antiproton impact. Present: (———) for proton, (– – –) for anti proton; Ford *et al* [39] (- - - - -) for electron removal; Chen *et al* [40] (–·–·–) for direct ionization.

In figure 4 we present our results for doubly differential cross sections as a function of electron ejection energy for 67 keV proton impact on atomic hydrogen. On comparison with the experiment of Kerby *et al* [41], we find the present results for variation of energy for the ejection angle of 50° agree reasonably well. However for the other angle, i.e. 30° there is some discrepancy with the experiment. In this case the present result shows a similar trend with the experiment, though it varies considerably with the increase of energy.

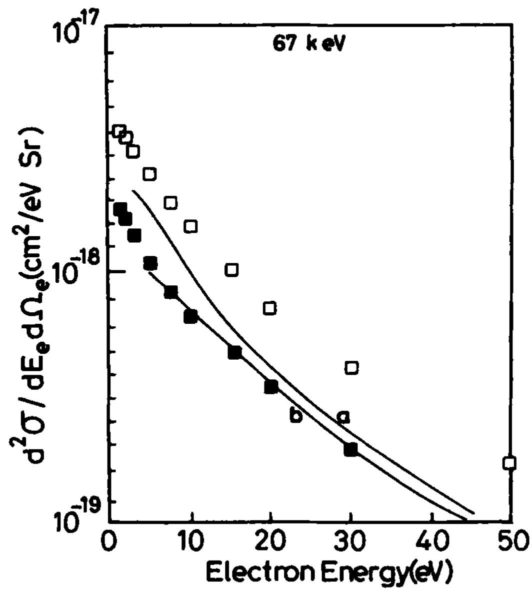

Figure 4. DDCS results for ionization of atomic hydrogen by 67 keV proton impact. Present (————); *a*: 30°, *b*: 50°. Experiment [34]: □ 30°, ■ 50°.

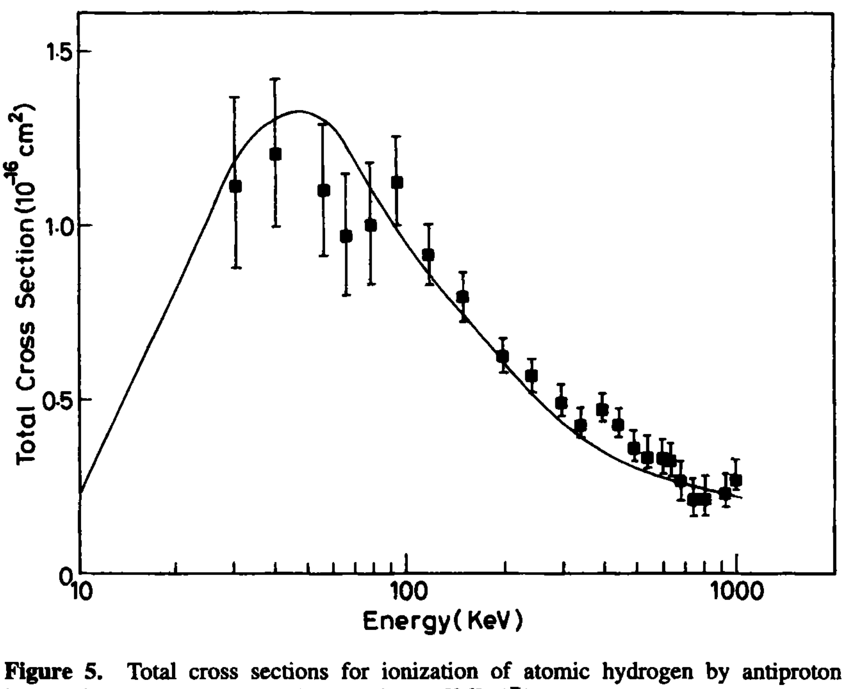

Figure 5. Total cross sections for ionization of atomic hydrogen by antiproton impact. Present: (————); Experiment [36]: (Ī).

In figure 5, the comparison of TICS is made between the recent experimental results of Knudsen *et al* [36] and the present calculated results for antiproton impact on atomic hydrogen in its ground state. We present here the results for several incident energies ranging from 10 to 1000 keV. The present results agree well with the experiment throughout the energy range considered. In the present case the maximum is observed at about 45 keV which is almost the same as the experimental result. The present curve shows a trend similar in nature to that of the experiment.

We compare our results with existing theoretical and experimental results. Our results for both proton and anti-proton impact agree well with experiments at intermediate and high energy region.

When we consider ionization we should note that in addition to ionization there are always possibilities of elastic scattering, excitation and charge transfer as well, in the ground state or in the excited states which influence the ionization cross sections, especially in the low energy region. Recently we proposed a theoretical method to calculate ionization cross sections in heavy particle collisions by impact parameter formalism. There we consider the influence of coupling with the important bound states in the direct as well as in rearrangement channels in a two centered atomic state expansion method. This work is in progress.

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